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NOVEL METHODOLOGY FOR APPLICATION OF ADAPTIVE SYSTEMS TECHNIQUES TO DMSP REMOTE TEMPERATURE SENSING

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Two new theoretical algorithms for the bias-free determination of atmospheric temperatures from upwelling radiance data were implemented in this research--the Differential Inversion (DI) algorithm and Optical Measure Theory (OMT). DI and OMT are complementary bias-free approaches to the construction of atmospheric temperature profiles. Previous work on DI at Creative Optics, Inc. was extended to permit the computation of partial atmospheric temperature profiles (at three altitudes) from Tiros Operational Vertical Sounder (TOVS) data. These partial temperature profiles demonstrated the utility of DI for the important operational problem of determination of the tropopause altitude. In OMT, atmospheric temperature profiles are the fundamental theoretical entities. Application of OMT to TOVS data in this research has resulted in the first bias-free computation of a complete atmospheric temperature profile from upwelling radiance data. This profile exhibits a meteorological character which is a natural consequence of the physical principles of radiative energy transfer on which OMT is based.

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Algorithmic studies in the development of DI and OMT have further elucidated the classic problems associated with the inversion of radiance data to obtain atmospheric temperature profiles. In both the DI and OMT algorithms, the numerical instabilities are now confined to a few well-characterized algorithmic steps amenable to treatment by specialized numerical techniques.

In addition to the TOVS data, data sets from the Defense Meteorological Satellite Program (DMSP) and ~~University of~~ Wisconsin's High-resolution Interferometer Sounder (HIS) were investigated for their suitability for inversion to atmospheric temperature profiles by DI and OMT .

ACKNOWLEDGMENTS

The following individuals were helpful to the authors in the course of this research. We wish particularly to acknowledge technical discussions with Dr. Jean I. F. King of the U.S. Air Force Geophysics Laboratory Atmospheric Sciences Division who was the Contracting Officer's Technical Representative. Dr. King provided great insight into the mathematical theories he developed which we subsequently implemented. Mr. Vincent Falcone, also of the AFGL Atmospheric Sciences Division, and alternate COTR, contributed important scientific assistance regarding analysis of atmospheric radiance data. Prof. Steven Leon of Southeastern Massachusetts University provided an informative exposition of the Nonlinear Hyperbolic Algorithm. The guidance and support of Dr. Robert McClatchey, Director of the AFGL Atmospheric Sciences Division is appreciated. Dr. Robert Knuteson of the University of Wisconsin has provided much useful information and assistance on the HIS data set, and Capt. Jill Smith of Global Weather Center supplied useful information regarding the DMSP database.

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EXECUTIVE SUMMARY

During the Phase I research effort, considerable progress was made in atmospheric temperature profile determination by extension of differential inversion (DI) techniques and the application of the Optical Measure Theory (OMT). These advances include the first-time-ever determination of partial atmospheric temperature profiles by application of the standard DI theory (first applied successfully to a single altitude by workers at Creative Optics, Inc.), and the first bias-free determinations of atmospheric temperature profiles by the application of OMT.

Phase I research demonstrated the applicability of the Nonlinear Hyperbolic Algorithm (NHA) and OMT to atmospheric profile determination and produced a successful temperature profile using these methods applied to TOVS data. See Figure 1. NHA/OMT are now well-characterized with regard to the numerical analytic properties relevant to practical implementation. As a result we now have a good theoretical understanding of the classic instability problems inherent to the inversion of upwelling radiances to obtain atmospheric temperature profiles. These instabilities are now localized to a few algorithmic steps within the NHA and are amenable to control by well understood numerical techniques. The behavior of the NHA in the presence of noise has been studied with a view ultimately to characterizing the information content of radiance data and the corresponding atmospheric structure parameters.

Determinations of partial atmospheric temperatures (three altitude points in the neighborhood of the tropopause) were also obtained using standard DI techniques by truncating the DI series at appropriate order. These partial profiles are of great interest in that they seem to replicate, faithfully, the actual temperature structure near the tropopause; this information is of great operational significance. See Figure 2.

The result of greatest immediate practical importance is the first successful determination of atmospheric temperature profiles using NHA/OMT. While still preliminary, these results are of great significance because:

- They are the first bias-free determinations of the earth's atmospheric temperature profile.
- They exhibit a meteorologic character; in particular, they correctly place the height of the tropopause when compared with radiosonde data.
- They demonstrate the theoretical validity of the NHA/OMT approach to atmospheric temperature profiling.

In addition to our successful utilization of TOVS data, two other two potential data sets for future analysis by DI and NHA/OMT techniques were analyzed and evaluated. Data from the Defense Meteorological Satellite Program (DMSP) microwave radiometer is reduceable using the same techniques we pioneered for TOVS, once data conversion and formatting problems are solved. An approach also has been developed for initial analysis of data from the High-Resolution Interferometer Spectrometer (HIS). HIS data poses new questions, and an opportunity to develop DI and NHA/OMT for new applications.

BIAS-FREE INVERSE TRANSFORMATION--
DEMONSTRATION ATMOSPHERIC TEMPERATURE PROFILE USING
OPTICAL MEASURE THEORY APPLIED TO TOVS DATA
(NONLINEAR LEAST SQUARES IMPLEMENTATION)

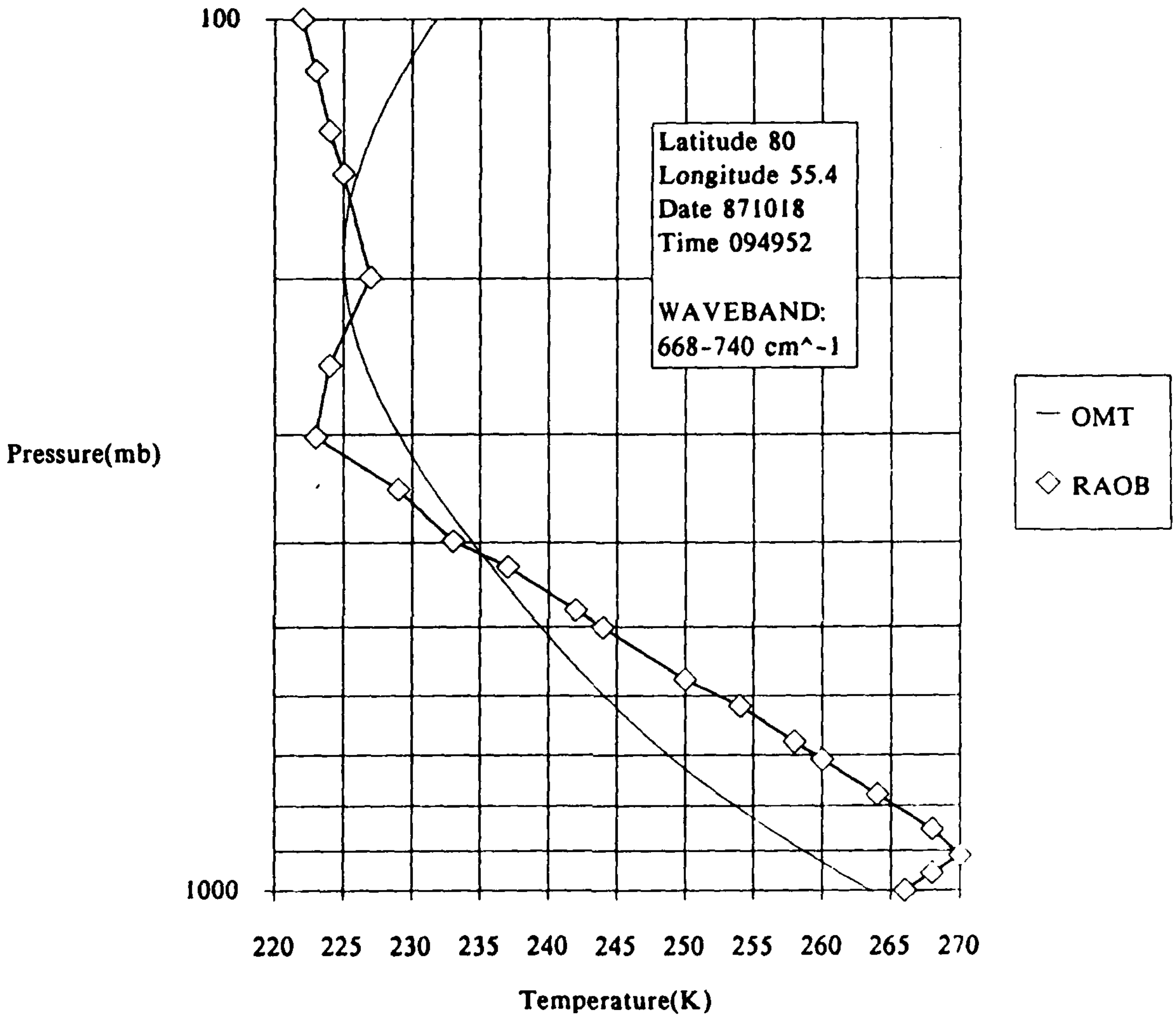

Figure 1. Bias-Free Inverse Tansformation. Researchers at Creative Optics, Inc. have produced the first bias-free atmospheric temperature profiles from satellite radiance data by an application of Dr. J. I. F. King's Optical Measure Theory (OMT). The profile shown here is obtained from data from the TIROS Operational Vertical Sounder (TOVS) which yielded six atmospheric structure parameters. The general meteorological character of the temperature profile is evident. High spectral resolution sounder data will permit calculation of more structure parameters to represent detailed features of the temperature profile.

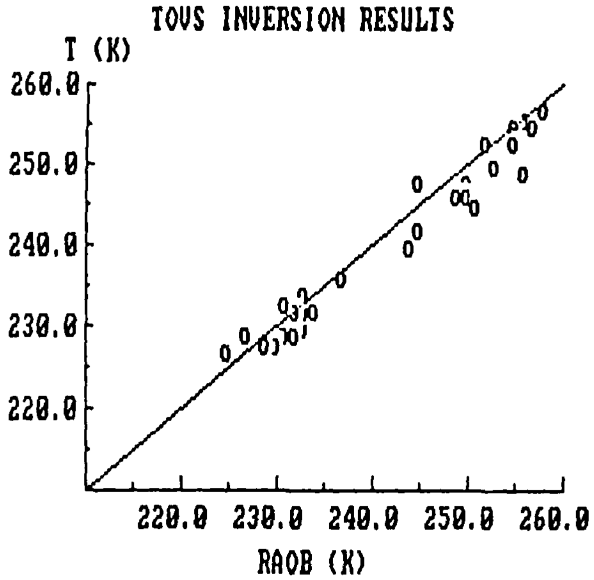

Figure 2a. TOVS Inversion Results. Researchers at Creative Optics have also produced the first multi-point temperature profile by application of Dr. J.I.F. King's Differential Inversion (DI) algorithm (implemented by Creative Optics, Inc. in a prior contract) to TOVS 4.3 μm data. Our results are plotted against temperatures obtained from RAOB data at 400 millibars (pressure/altitude).

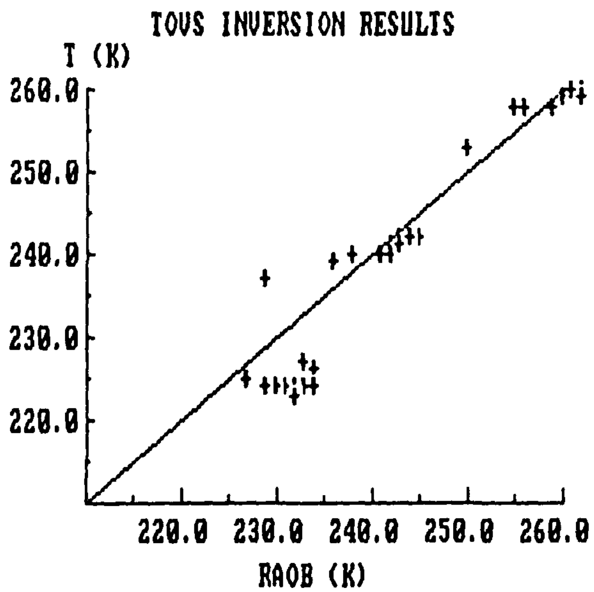

Figure 2b. TOVS Inversion Results. We have also applied the DI algorithm to 15 μm TOVS data for atmospheric temperature values at 400 millibars. Slightly larger errors are apparent on the long wavelengths, but the correspondence with RAOB measurements is still good.

1. INTRODUCTION

1.1 **Background**. Satellite observations provide the only practical means of obtaining temperature profiles in the atmosphere over large geographic areas (especially over oceans) and over long periods of time. This implies that the development of new and computationally effective algorithms for measuring atmospheric temperature profiles from satellite data is a significant and important task.

The measurable quantity most accessible to satellite observations is the infrared upwelling radiance. Most typically this is measured at wavelength ~ 15 μm near the atmospheric CO_2 absorption band. Different spectral regions in this wavelength region become optically thick at different heights in the atmosphere, and so the upwelling infrared radiance in those wavelength intervals contains, at least in principle, information about the Planck function at different heights in the atmosphere. On this basis, one should be able to determine a temperature profile of the atmosphere using measurements of the upwelling infrared radiance.

In practice, we must solve the radiative transfer equation for the Planck function over this spectral interval, a Fredholm integral equation of the first kind. Since we are dealing with an integral equation, we must cope with problems of non-uniqueness of the solution obtained. This is a problem of practical importance because the range of plausible solutions of the transfer equation (within limits imposed by the accuracy of the experimental data) cover an unacceptably large range of temperatures.

A number of workers have approached this problem with techniques designed to obtain the "true" temperature profile (or at least a pragmatically useful profile) by a variety of methods, most of which require some *a priori* assumptions such as an initial temperature profile. Application of relaxation techniques (Chahine 1970, 1972; Smith 1970;Yeh, Vonder Haar, and Liou 1985) requires the selection of an initial temperature profile to commence an iterative process. Application of the method of Backus and Gilbert (Conrath 1972) requires the assumption of a reference temperature profile in order to evaluate radiative transfer kernels.

Other relevant work has been undertaken (Twomey 1970) to delineate the limits in information content of solutions of the radiative transfer equation. In this vein, Fourier analysis of the radiative transfer equation (Gautier and Revah 1975) allows treatment of the temperature profile as a band-limited spectrum.

In this report we consider new approaches to this problem based on Laplace transform theory (King, Hohlfeld and Killian (1988); King 1983, 1985; Leon and King 1988)--Differential Inversion (DI) and Optical Measure Theory (OMT). The techniques use the upwelling radiance measurements and their logarithmic pressure derivatives to construct an atmospheric temperature profile. The methods have the particular theoretical attraction of assuming no *a priori* information about the temperature profile beyond the fact that it is reasonably smooth (*i.e.* analytic). Our numerical studies and simulations using the algorithms have investigated the viability of these approaches and indicated some of their sensitivities to truncation error, roundoff error, experimental uncertainty, and other noise processes. DI and OMT have been successfully applied to a sample of data from the NOAA TIROS Operational Vertical Sounder (TOVS).

1.2 **Phase I Technical Objectives**. Broadly speaking the work undertaken during the Phase I research effort was directed toward adapting existing software for determination of atmospheric temperature profiles by DI to the specific application of the reduction of radiance data. Not only did we achieve our original objectives, we achieved successes in new areas not originally proposed, viz., new software developed for the implementation of the OMT and the Nonlinear

Hyperbolic Algorithm (NHA) which permits computation of bias-free atmospheric temperature profiles from radiance data.

2. PARTIAL ATMOSPHERIC TEMPERATURE PROFILES BY DIFFERENTIAL INVERSION

The differential inversion algorithm of King (1988) has been applied by research workers at Creative Optics, Inc. to obtain the first bias-free determinations of atmospheric temperature (King, Hohlfeld, and Kilian 1988). The first such application used seven channels of 4.3 μm infrared data from the Tiros Operational Vertical Sounder (TOVS) instrument to obtain a single temperature value at 398 millibars.

Temperature values in the differential inversion theory are expressed in terms of a series expansion involving the radiance and radiance derivatives,

$$B(z) = \sum_{k=0}^{\infty} \lambda_k D^{(k)} R(\zeta) \tag{1}$$

where B is the Planck function, R is the radiance, $z = -\ln P$, where P is the pressure at which the weight function reaches its maximum value, and $\zeta = -\ln p$ is a height-like variable where p is barometric pressure. The λ_i's are the differential inversion coefficients determined as moments of the weight functions. Originally, all seven TOVS channels were employed to obtain radiance numerical derivatives via centered divided differences out to the third derivative (i.e. the term containing λ_4), which permitted the evaluation of a single atmospheric temperature value at the central P value among the seven channels, as shown in Figure 2.

It was noted, however, that convergence of this series was very rapid, and the contribution of the highest order terms was less than the expected errors arising due to numerical and experimental sources of error. Therefore, we truncated the differential inversion series at second order, so that two additional atmospheric temperature values could be obtained, while still computing all numerical derivatives as centered divided differences (Hohlfeld, Kilian, Drueding, and Ebersole 1988). These additional temperature points were obtained at pressure values of 174 and 661 millibars, as shown in Figure 3.

A collection of Zone 1 (latitude = 60° N to 90° N) TOVS data were analyzed in this fashion and the results are collected in Appendix A. It may be seen by comparison with the RAOB data, that significant atmospheric structure has been represented by these preliminary results. Most notably, data points on either side of the tropopause have been obtained, demonstrating the potential utility of this analysis technique for satellite remote measurement of the altitude of the tropopause.

DIFFERENTIAL INVERSION APPLIED TO TOVS DATA TO OBTAIN A THREE POINT PROFILE

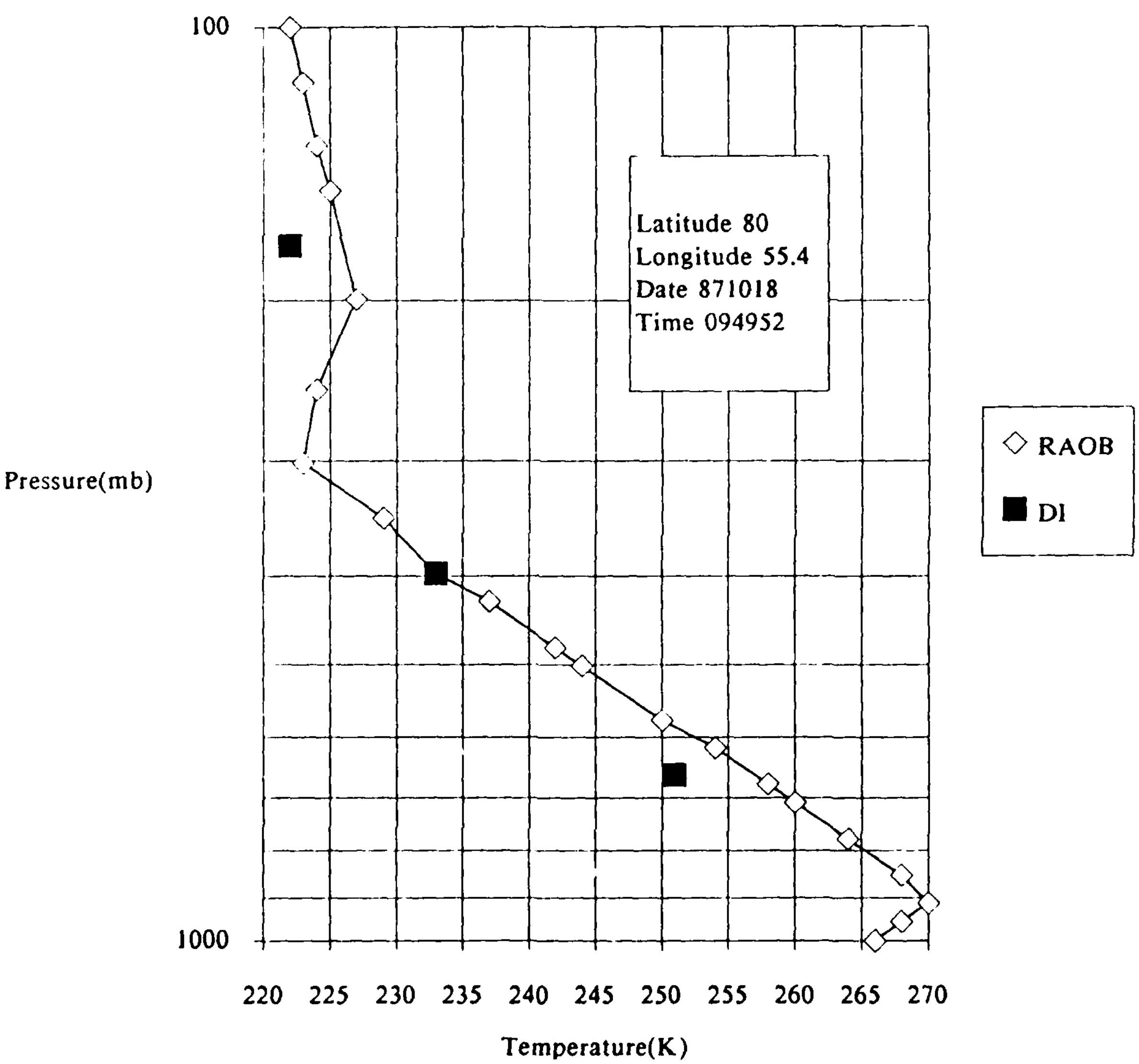

Figure 3. Differential Inversion Applied to TOVS Data to Obtain a Three-Point Temperature Profile. Shown here is a representative example of Creative Optics' results for partial atmospheric temperature profiles (at three altitudes) from 4.3 μm to TOVS data. Note that temperature values on either side of the tropopause have been obtained. This demonstrates the potential ability of this algorithm for the important operational problem of determination of tropopause altitude by remote sensing. Other examples are presented in Appendix A.

3. OPTICAL MEASURE THEORY

3.1 Introduction. Optical Measure Theory (OMT) is a theoretical approach to the problem of determination of atmospheric temperatures in which an atmospheric temperature profile is the fundamental theoretical object. That is to say, OMT is formulated in terms of atmospheric temperature profiles in the same sense as DI is formulated in terms of obtaining discrete temperature values in the atmosphere.

OMT has been developed on the basis of advances in transform theory (Leon and King 1988, King 1988). Specifically it was noted by King that the radiative transfer equation represents a generalization of the Laplace transform, in the manner that it relates the Planck function profile to the radiance profile. Based on this insight, it is then natural to represent the radiance profile in some appropriate functional form (the selection of the appropriate functional form is a problem discussed below) and then to compute the Planck function profile, and hence the atmospheric temperature profile, as an inverse transform of the radiance profile.

Several important advantages derive from this approach. First of all, temperature profiles arise in a natural manner in OMT. Secondly, if an intelligent choice is made regarding the functional representation of the radiance data, these profiles will necessarily exhibit a meteorological character. Lastly, and perhaps of the greatest importance, the classical numerical instability of the atmospheric radiance inversion problem is localized algorithmically to a few well-understood steps which may then be treated with specialized techniques.

3.2 Theoretical Development of Optical Measure Theory. For sake of completeness, we shall derive here the fundamental equations of OMT. Following King (1988) and Leon and King (1988), we note that the equation for upwelling radiance

$$R(\mu) = \int_0^\infty B(p)W(p/\mu)\,\frac{dp}{p} \tag{2}$$

has the character of an integral transform from B(p), the Planck function as a function of pressure, p, to the radiance, $R(\mu)$, where μ is a pressure-like transform variable. Here $W(p/\mu)$ is the usual atmospheric weight function. In the context of the standard DI development, μ, would be viewed as that pressure value at which the weight function achieved its maximum value. If the actual atmospheric weight function is well-represented as a generalized exponential function (King 1985; King, Hohlfeld, and Kilian 1988)

$$W(p/\mu) = W_m(p/\mu) = \frac{m^m}{\Gamma(m+1)}(p/\mu)\ \exp[-m(p/\mu)^{1/m}], \tag{3}$$

then for m = 1, Eq. (2) immediately assumes the character of a Laplace transform,

$$R(\mu) = \frac{1}{\mu}\int_0^\infty B(p)e^{-(p/\mu)}\,dp \tag{4}$$

i.e. $\mu R(\mu)$ is the Laplace transform of B(p) with respect to the transform variable $1/\mu$. When $m \neq 1$, the radiance profile and Planck function profile are then related by a generalization of the Laplace transform defined in terms of the generalized exponential function. (For example with TOVS data see Figure 4.) All of the useful analytic properties of the Laplace transform are retained in this generalization of the Laplace transform utilizing the generalized exponential function kernel.

If a choice of functional form is made for B(p) (or alternatively $R(\mu)$), Equation (2) then immediately implies the functional form $R(\mu)$ (alternatively B(p)). This observation is especially pertinent if we note that the Planck function profile of a radiative atmosphere is exponential in form, i.e.

$$B(p) = Le^{-kp} \tag{5}$$

with k and L constants (Chandrasekhar 1960). The corresponding (m = 1) radiance profile function is then,

$$R(\mu) = \frac{L}{1 + k\mu} \tag{6}$$

This discussion motivates a choice of the functional form by which radiance data is represented (King 1988; Leon and King 1988),

$$R(\mu) = a + b\mu + \sum_{i=1}^{j} \frac{L_i}{1 + k_i\mu} \tag{7}$$

where j hyperbolic terms are included. The addition of a linear term of form $a + b\mu$ (with a and b constants) was found by Leon and King to be of practical utility in the representation of radiance data. Generalization to the inclusion of a polynomial of arbitrary order in μ is straightforward. The corresponding Planck function profile obtained by generalized inverse Laplace transformation (for arbitrary m) of Eq. (7) is

$$B(p) = a + bp + \sum_{i=1}^{j} L_i E_m(-k_i p) \tag{8}$$

where $E_m(x)$ is the generalized exponential function with parameter m.

The choice of an exponential (or generalized exponential form of the Planck function profile, motivated by the expectation of the real atmospheric acting at least in part as a radiative atmosphere, indicates that Eq. (8) is a natural choice of functional form for the representation of radiance data.

3.3 The Nonlinear Hyperbolic Algorithm. The theoretical discussion given above shows the importance of fitting upwelling radiance data to a functional form as given in Eq. (7). Leon and King (1988) have developed an algorithm, the Nonlinear Hyperbolic Algorithm (NHA), for fitting radiance data to a formula of the form of Eq. (7). As such, NHA is the natural starting point for any discussion of the properties of the OMT. The NHA allows determination of the constants a, b, and the set of L_i's and k_j's in Eq. (7), which then immediately determines the corresponding terms of the Planck function profile, given by Eq. (8), and hence the atmospheric temperature profile.

We now outline the steps of the NHA. Assume that we are given 2n = 2j + 2 upwelling radiance measurements, which are to be fitted to a formula of the form of Eq. (7), i.e., we wish to determine a, b, L_1, ..., L_j, k_1, ..., k_j, a total of 2n constants from 2n radiance measurements. Following Chandrasekhar (1960), the radiance is represented as a rational function in μ,

$$R(\mu) = \frac{d_1 + d_2\mu + \ldots + d_{n+1}\mu^n}{d_{n+2} + d_{n+3}\mu + \ldots + d_{2n}\mu^{n-2} + \mu^{n-1}} = P(\mu)/Q(\mu). \tag{9}$$

This should be viewed as a linear system of equations for the d_i's of rank 2n. Writing this system as $P(\mu_i) = Q(\mu_i)R_i$ where μ_i is the pressure of the weight function maximum of the ith channel, we obtain 2n equations for the 2n unknowns, where the ith equation is

$$d_1 + d_2\mu_i + \ldots + d_{n+1}\mu_i^n - R_i d_{n+2} - R_i d_{n+3}\mu_i - \ldots - R_i d_{2n}\mu_i^{n-2} = \mu_i^{n-1}R_i \tag{10}$$

This linear system may be solved by any of the standard techniques for linear systems of equations, such as singular value decomposition (Press, Flannery, Teukolsky, and Vetterling 1986). Matching orders for μ^0 and μ^1 in Eqs. (9) and (7), we obtain

$$\begin{aligned} b &= d_{n+1} \\ a &= d_n - d_{n+1}d_{2n} \end{aligned} \tag{11}$$

The remaining coefficients in Eq. (7) may be determined by noting that the locations of poles in $R(\mu)$ determine values of the k_j's.

$$k_j = -1/c_j \tag{12}$$

where c_j is the jth root of $Q(\mu)$. The roots of $Q(\mu)$ may be found by any of the standard root-finding applicable to polynomials, such as the Laguerre method (Press, Flannery, Teukolsky, and Vetterling 1986), which allows for the presence of complex roots. Lastly, the L_j values may be determined by solution of the linear system of equations

$$\sum_{j=1}^{n} \frac{L_j}{1+k_j\mu_j} = R_j - a - b\mu_j \tag{13}$$

where $j = 1, \ldots, n$ is any subset of the radiance measurements.

3.4 <u>Stability of the Nonlinear Hyperbolic Algorithm</u>. While the NHA is well-grounded on physical principles applicable to radiative transport in the earth's atmosphere, practical difficulties arise in the numerical stability of the NHA. Determination of the coefficients in Eq. (7) in application of the NHA is analogous to a classic problem in curve-fitting, that of fitting exponential curves to radioactive decay data of several radionuclides, well-known to be numerically unstable (Acton 1970). This may be seen qualitatively by noting that e^{-x} and $1/(1+x)$ are roughly equal over the range $0 < x < 1$.

These numerical instabilities manifest themselves as an ill-determinedness in applications to radiance data of the NHA coefficients a, b, $k_1, \ldots k_i$, $L_1, \ldots L_i$. Small perturbations of the input radiance values lead to large changes in the coefficients of the fit determined by the NHA.

It is instructive to note that the transformation of the radiance series, Eq. (7), to the Planck function series, Eq. (8), is absolutely stable. Furthermore, obtaining the temperature profile from the Planck function profile involves a stable and continuous transformation. Therefore, all of the classical numerical instability of the problem of determination of the atmospheric temperature profile from upwelling atmospheric radiances has been localized algorithmically in the NHA. In particular, the principal unstable operations in the NHA involve the solution of the linear system for the coefficients $d_1, \ldots, d_{2n}$. It is of great practical significance in applications to inversion problems to fully understand the origin of numerical instabilities in order to control them effectively by specialized numerical techniques.

3.5 <u>Implementation of the Nonlinear Hyperbolic Algorithm and Analysis of Its Numerical Stability Properties</u>. Creative Optics, Inc. has carried out a successful implementation of the NHA in the FORTRAN language running on PC-AT class microcomputers. Previous implementations by Leon and King (1988) utilized a PC-based MATHCAD package suitable for exploratory work, while the FORTRAN-based implementation discussed here represents a significant step towards an efficient, operational of the NHA.

Several specialized numerical techniques were employed to optimize the numerical stability properties of the NHA. Most important is the use of singular value decomposition (Press, Flannery, Teukolsky, and Vetterling 1986) for the solution of the linear system determining the coefficients $d_1, \ldots, d_{2n}$. Singular value decomposition is useful for the solution of ill-conditioned linear systems because it is capable of returning partial solutions if the quality of the data set will not permit a well-conditioned solution of full rank.

Solution for the roots of the polynomial equations for the k_i's was carried out by Laguerre's method (Press, Flannery, Teukolsky, and Vetterling 1986). Laguerre's method is able to compute complex polynomial roots as effectively as real roots, and its convergence to roots is guaranteed. When combined with standard decimation-in-order techniques, Laguerre's method is an effective approach to root-finding of polynomials, even polynomials of moderately large order.

Studies were undertaken using this FORTRAN implementation of the NHA to characterize the numerical stability of the NHA in controlled computational experiments. These studies involved applying the NHA both to synthetic radiance values generated from integration of the radiative transfer equation, supplied with a realistic atmospheric temperature profile, and with radiance values generated by application of Eq. (7) with known coefficients. These values may be computed with known values of Gaussian noise so as to determine the sensitivity of the NHA to experimental errors.

Studies have been undertaken to investigate the sensitivity of the NHA both to noise in the radiance amplitudes and noise in the P values, i.e. uncertainty in the pressure value at which the corresponding channel weight functions achieve their maximum values. These latter sources of error were motivated by noting practical difficulties experienced in fitting generalized exponential functional forms to some atmospheric weight functions. This implies, in effect, that some P values are not well-determined at the 5% level.

During the Phase I effort we have obtained a preliminary quantification of the level of sensitivity of the NHA to experimental noise. The NHA still functions reliably and effectively in the presence of Gaussian noise in radiance values at the 5% to 10% level. It is interesting and significant to note that the NHA is comparatively sensitive, however, to noise in the P values. Noise in excess of 1% in P may prevent the NHA from finding physically meaningful coefficients for the nonlinear hyperbolic fit. This result highlights the importance of the techniques we have developed at Creative Optics for the analysis of atmospheric weight functions, which can now be seen to be of significance for the practical application of the NHA.

We have characterized the behavior of the NHA under these circumstances which are numerically ill-conditioned due to the presence of experimental errors. Typically negative values of the k_i's are obtained, which correspond to poles in the radiance formula at positive values of pressure, or values of k_i's which are complex conjugate pairs. Clearly, both of these cases correspond to nonphysical solutions and are readily identified as such. This error-checking feature is important for an operational algorithm which must perform reliably in the presence of occasional bad data.

Leon and King (1988) have demonstrated the utility of the NHA for detecting spurious values in radiance data corrupted by a single bad channel. Our studies confirm the ability of the NHA to detect the corrupted channel and to generate the best possible fit to the remaining radiance data when the bad channel value is ignored. We have furthered these studies by considering experimental errors in which each channel is degraded by some level of random noise. Under these circumstances, when the noise level in the radiances reaches the 5% to 10% level (as discussed above) the values of the k_i's become poorly determined (due to loss of numerical condition of the NHA) and poles are introduced in apparently random locations in pressure space. This behavior should be contrasted with the behavior elucidated by Leon and King where the pole occurs at a definite location in proximity to the single spurious channel.

It is important to note that the fundamental results of this study relative to the sensitivity of the NHA to uncertainty in P values and the behavior of the NHA in the presence of noise now permit practical application of the NHA under realistic conditions. This is especially true when the atmospheric weight functions are well-determined and functionally well-characterized.

4. NONLINEAR LEAST SQUARES NONLINEAR HYPERBOLIC ALGORITHM

4.1 Motivation and Theoretical Development. Algorithmic extension of the NHA was considered as a means of coping with the inherent numerical instability of the NHA. It is desirable to retain the functional form of Eq. (7) as an appropriate representation of radiances from a radiative atmosphere, however, this choice of hyperbolic functions is the ultimate origin of the numerical instability of the NHA. The numerical instability of the NHA may be viewed as arising when the information content of the radiance data set is insufficient to determine all the coefficients in the nonlinear hyperbolic representation. A strategy suggested by this observation is to attempt to fit a limited set of hyperbolic terms, in a least-squares sense, to the available radiance data.

In the Phase I research effort carried out at Creative Optics, Inc., we have implemented an extension of the NHA based on nonlinear least-squares (NLLS) techniques. As presently implemented, the NLLS NHA is a test-bed algorithm used to investigate detailed approaches for developing fits of the form of Eq. (7) to radiance data.

The NLLS NHA is carried out by the standard Levenburg-Marquardt algorithm (Press, Flannery, Teukolsky, and Vetterling 1986). In typical operation of the NLLS NHA, a fit is made to the linear terms (determination of a and b) and a single hyperbolic term (determination of L_1 and k_1). Successive hyperbolic terms are added until a nonphysical term is obtained (i.e. with a negative k value), which is then discarded and the NLLS NHA algorithm is then terminated.

4.2 Initial Results from the NLLS NHA. During the Phase I research effort at Creative Optics, Inc., the NLLS NHA was applied to a few TOVS Zone 1 measurements and a successful inversion of TOVS radiance data to yield an atmospheric temperature profile was obtained. Six TOVS channels (1, 2, 4, 5, 6, 7) were used to obtain the results shown in Figure 1. This profile has an evident meteorological character, particularly in that a minimum in the atmospheric temperature profile approximately at the tropopause altitude is seen. It is also evident that the NLLS NHA generates the smoothest radiance profile consistent with the observed radiance data. This is a highly desirable feature in that the simplest possible atmospheric temperature profile is constructed. Atmospheric structure not supported by the radiance data is not "invented" by the algorithm. The six atmospheric structure parameters determined (a, b, k_1, L_1, k_2, L_2) do not contain sufficient information to represent detailed structures in the atmospheric temperature profile such as the ground-level temperature inversion seen in the radiosonde data corresponding to this temperature profile in Figure 1. It is expected that application of the NLLS NHA to temperate latitude (Zone 2) TOVS data will be more successful in terms of detailed matches between radiosonde data and temperature profiles derived by the NLLS NHA. The preliminary result shown here demonstrates the potential practical utility of the NLLS NHA, particularly for the important problem of remote-sensing of the tropopause altitude.

4.3 Recommended Upgrades to the NLLS NHA, Choice of Basis Functions, and Determination of Atmospheric Structure Parameters. The performance of the present version of the NLLS NHA is limited by the geometry of the χ^2 (error) surface. NLLS algorithms attempt to determine a set of parameters of a functional fit corresponding to a (global) minimum in χ^2. However, if the error surface has many secondary (local) minima, it is possible for the NLLS algorithm to return a solution corresponding to one of these secondary minima in χ^2 rather than the true global minimum corresponding to the desired physical solution. Such irregular error surfaces are characteristic of ill-conditioned curve fitting problems (Acton 1970).

Standard techniques have been developed for nonlinear least-squares curve fitting under such circumstances. These techniques include grid search, Monte Carlo methods, addition of numerical "momentum" terms to NLLS, conjugate gradient search on the χ^2 surface, and others.

Choice of an appropriate method is best made after a more detailed characterization of the geometric properties of the χ^2 surface, which is appropriate to a Phase II effort. Application of such techniques can be expected to make determination of coefficients of an NHA fit routine and completely independent of all starting values used to initiate the NLLS NHA fit.

Determination of the NHA parameters can be viewed as the determination of a set of atmospheric structure parameters that may be used to represent corresponding structure in the atmospheric temperature profile. Since, at most, only as many structure parameters may be obtained as the number of channels in the original radiance data, it is clear that fundamental theoretical limits exist as to the amount of atmospheric structure which can be represented on the basis of a given radiance data set. Furthermore, if the channel measurements of radiance are not all statistically independent, information theoretical principles suggest that only a smaller number of NHA parameters may be consistently obtained.

These considerations on the information content of radiance data and their translation into atmospheric structure parameters by NHA/OMT suggest exciting possibilities for the design of temperature sounding instruments which can be optimized to represent structure in the atmospheric temperature profile with specified resolution in height. In addition to the production of atmospheric temperature profiles as such, this represents an important practical advance of NHA/OMT.

The preliminary research carried out at Creative Optics, Inc. during Phase I indicates the importance of numerical condition and numerical stability both for NHA and to a lesser extent for NLLS NHA. The choice of hyperbolic functions to represent radiances is well-motivated by the physics of the atmosphere, however, it is also well-known that not all energy transport in the earth's atmosphere is radiative. During the Phase II research effort, additional basis functions should be investigated for the representation of radiance data. While the use of hyperbolic functions as a part of the NLLS NHA fitting procedure should be retained. addition of new basis functions will change the geometry of the χ^2 surface. This will yield improvements in the numerical condition of the NLLS NHA and improve its efficiency for the determination of global minima in the χ^2 surface corresponding to physically meaningful atmospheric temperature profiles.

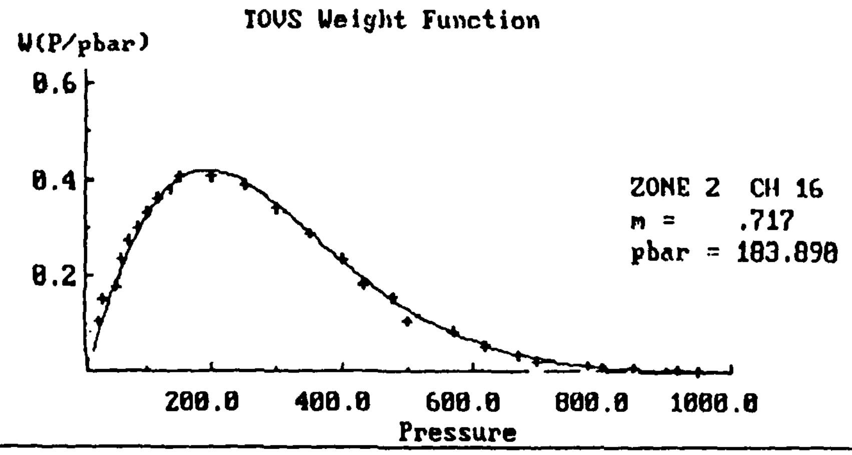

Figure 4. TOVS Weight Function. We found in our work with King's Differential Inversion algorithm that atmospheric weight functions are well represented by generalized exponential weight functions shown here (solid line) for m=0.742 and P=180.085 millitors, plotted together with the weight function for TOVS channel 16 (crosses).

5. DATA ANALYSIS AND DATA EVALUATION

5.1 Introduction. During the Phase I research effort we have been concerned with obtaining and/or evaluating suitable radiance data sets for continued development, testing, and evaluation of extensions of the DI algorithm and development of NHA/OMT. This establishes a foundation for the Phase II effort which will be directed towards developing DI and NHA/OMT algorithms to a state suitable for the routine reduction of radiance data to atmospheric temperatures and atmospheric temperature profiles.

5.2 TOVS. To date, data from the Tiros Operational Vertical Sounder (TOVS) has been the principal resource for the development and testing of DI and NHA/OMT algorithms. TOVs data is currently available in-house at Creative Optics, Inc. with 15 scans with corresponding radiosonde data in each of three latitude zones, Zone 1 (polar, latitude = 60° N to 90° N), Zone 2 (temperate, latitude = 30° N to 60° N), and Zone 3 (equatorial, latitude = 0° N to 30° N).

A summary of TOVS instrumental characteristics is given in Table 1. Additional TOVS data is readily obtainable for support of the Phase II research effort. [For further relevant information on TOVS, see (NOAA 1983; Smith et al. 1979; Weinreb et al. 1981) and references cited therein.]

TABLE 1. Summary of TOVS Instrumental Characteristics.

TOVS Channel #	Central Wavenumber(cm^{-1})	P(mb) (zone 1)	Half-power bandwidth(cm^{-1})
1	668	25.9	3
2	679	69.5	10
3	691	85.	12
4	704	400.	16
5	716	543.	16
6	732	780.	16
7	748	1000.	16
13	2190	992.	23
14	2213	663.	23
15	2240	400.	23
16	2276	172.	23
17	2361	25.9	23

5.3 HIS. Data were obtained from the High-resolution Interferometer Sounder (HIS) developed by researchers at the University of Wisconsin. (See Revercomb et al 1988.) HIS is a Fourier-transform spectrometer operating between 509 cm^{-1} and 2750 cm^{-1}. Relevant characteristics of the HIS instrument are given in Table 2. A set of 15,000 radiances and corresponding weight functions have been obtained from HIS and a significant subset of them have been examined. The most notable qualitative difference between the HIS data and the other data sets we have examined is that the HIS weight functions exhibit multiple maxima. (See Figure 5a for a representative example.) These weight functions arise due to the contributions of chemical species in addition to carbon dioxide. DI and NHA/OMT will require some generalization in order to reduce radiance data such as these. Until such theoretical generalization is accomplished, reduction of HIS data will be restricted to those wavelength intervals where only absorption of a single species is important, so that the weight function corresponding to that wavelength interval exhibits a single well-defined maximum. (See Figure 5b for an example.) Sufficient wavelength coverage is expected, even with that restriction, to achieve a high vertical resolution atmospheric temperature profile.

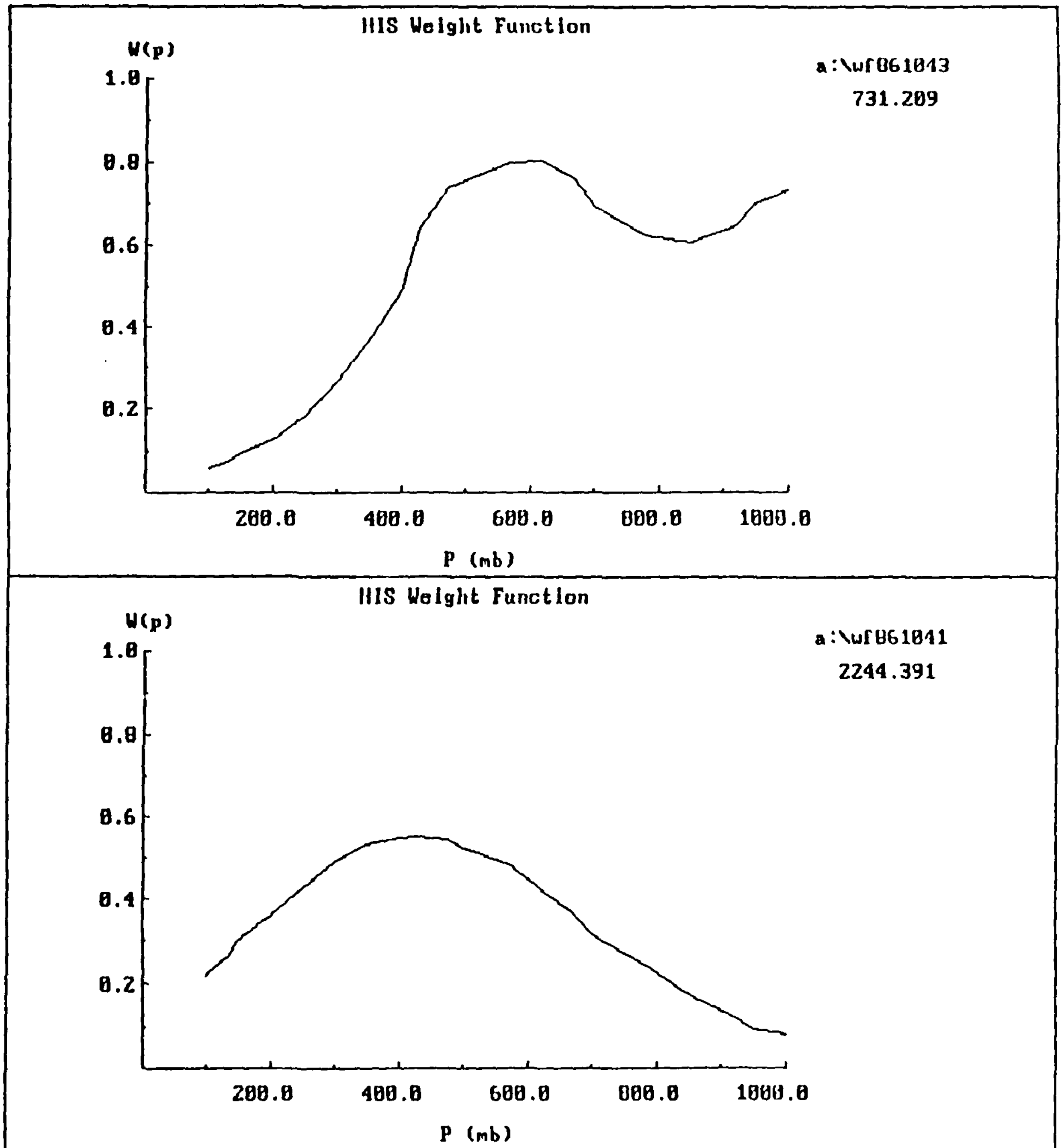

Figure 5. HIS Weighting Functions. Two representative weight functions for the High-resolution Interferometer Sounder (HIS) developed by the University of Wisconsin. The weight function in (a) exhibits multiple maxima due to multiple chemical gaseous species contributing to atmospheric absorption at wavelength frequency of 731.209cm^{-1}. The single peak in (b) corresponds to a wavelength interval (centered at 2244.391cm^{-1}) that exhibits a single well-defined maximum.

TABLE 2. Summar of HIS Instrumental Characteristics.

HIS	(Unapodized) Resolution
Band I 590-1070 cm^{-1}	.364 cm^{-1}
Band II 1040-1930 cm^{-1}	.641 cm^{-1}
Band III 2070-2750 cm^{-1}	.641 cm^{-1}

5.4 DMSP. The Defense Meteorological Satellite Program (DMSP) satellites carry a six-channel microwave radiometer for atmospheric temperature sounding. The relevant characteristics of this instrument are listed in Table 3. On the basis of the instrumental characteristics of DMSP and published weight functions, we anticipate that reduction of DMSP by DI or by NHA/OMT will be analogous to the reduction of TOVS data. DMSP data could not be obtained during the Phase I effort because radiances are only available from Global Weather Central at Offut Air Force Base in a 36 bit format (as required for management of the DMSP database by Sperry-Univac computers used at Global Weather Central). Data can be made available after a time of three to four months from the time of request, which is the time required for a data translation program to be made by workers at Global Weather Central.

TABLE 3. Summary of DMSP Instrumental Characteristics.

DMSP Channel #	Peaking Height(km)	Frequency (GHz)	Bandwidth (MHz)	NETD (K)	Calib Uncertainty(K)
1	0	50.5	400	0.32	0.25
2	2	53.2	400	0.24	0.21
3	6	54.35	400	0.36	0.24
4	10	54.9	400	0.22	0.13
5	30	58.4	115	0.39	0.06
6	16	58.825	400	0.29	0.24
7	22	59.4	250	0.31	0.13

6. CONCLUSIONS

A number of conclusions can be drawn from this research relevant to the construction of atmospheric temperature profiles from upwelling radiance data:

6.1 Differential Inversion (DI).

• When the series representation of the Planck function is rapidly convergent, DI can yield multiple atmospheric temperature values suitable for the construction of partial atmospheric temperature profiles.

• The partial temperature profiles determined from DI are suitable for bias-free determination of significant meteorological structures, such as the height of the tropopause.

• DI is well-suited to radiance data sets in which the channel weight functions sample the atmosphere finely in pressure.

6.2 Optical Measure Theory (OMT) and Nonlinear Hyperbolic Algorithm (NHA).

• The OMT with its principal algorithmic element, the NHA, have been implemented in an effective FORTRAN program as a significant step towards eventual operational implementation of these algorithms.

• The algorithmic properties of the NHA for uniformly noisy radiance data and for radiance data in which only single channels are corrupted by errors have been characterized. The ability of the NHA to adaptively process radiance data with single corrupt channels, noted by Leon and King, has been confirmed by our work.

• The importance for NHA of uncertainties in pressure values at which atmospheric weight functions achieve their maximum values has been determined.

• Numerical instability of the NHA is now well-characterized and understood in its relation to the overall stability of the classic problem of inversion of radiances to atmospheric temperatures.

6.3 Nonlinear Least Squares (NLLS) Extension of NHA.

• A nonlinear least-squares extension of the NHA has been demonstrated and shown to be an appropriate strategy for generating as many hyperbolic terms in the NHA as the data will support.

• Improvement of the NLLS NHA can be expected as a result of application of standard algorithmic techniques appropriate to least-squares curve-fitting when the error surface exhibits multiple secondary minima.

6.4 OMT and DI: Bias-Free Determination of Atmospheric Temperature Profiles.

• OMT has demonstrated the generation of a bias-free atmospheric temperature profile from TOVS data. This profile exhibits a meteorological character, in particular, showing a temperature minimum in temperature at the tropopause altitude.

• The algorithmic basis of OMT, from transform theory, is the correct approach to the calculation of atmospheric temperature profiles. The temperature profiles obtained are the smoothest bias-free temperatures consistent with the radiance data.

• DI and OMT are complementary bias-free approaches to the determination of atmospheric temperatures from upwelling atmospheric radiances. (See Figure 6.) DI calculates temperatures at some set of pressure values in the atmosphere with no underlying assumption regarding the functional form of the radiance data. OMT is fundamentally oriented towards the production of a temperature profile, but implicitly assumes that the dominant mode of energy transport in the atmosphere is radiative. Additional research will elucidate the relative merits of these two novel approaches to remote sensing of atmospheric temperatures.

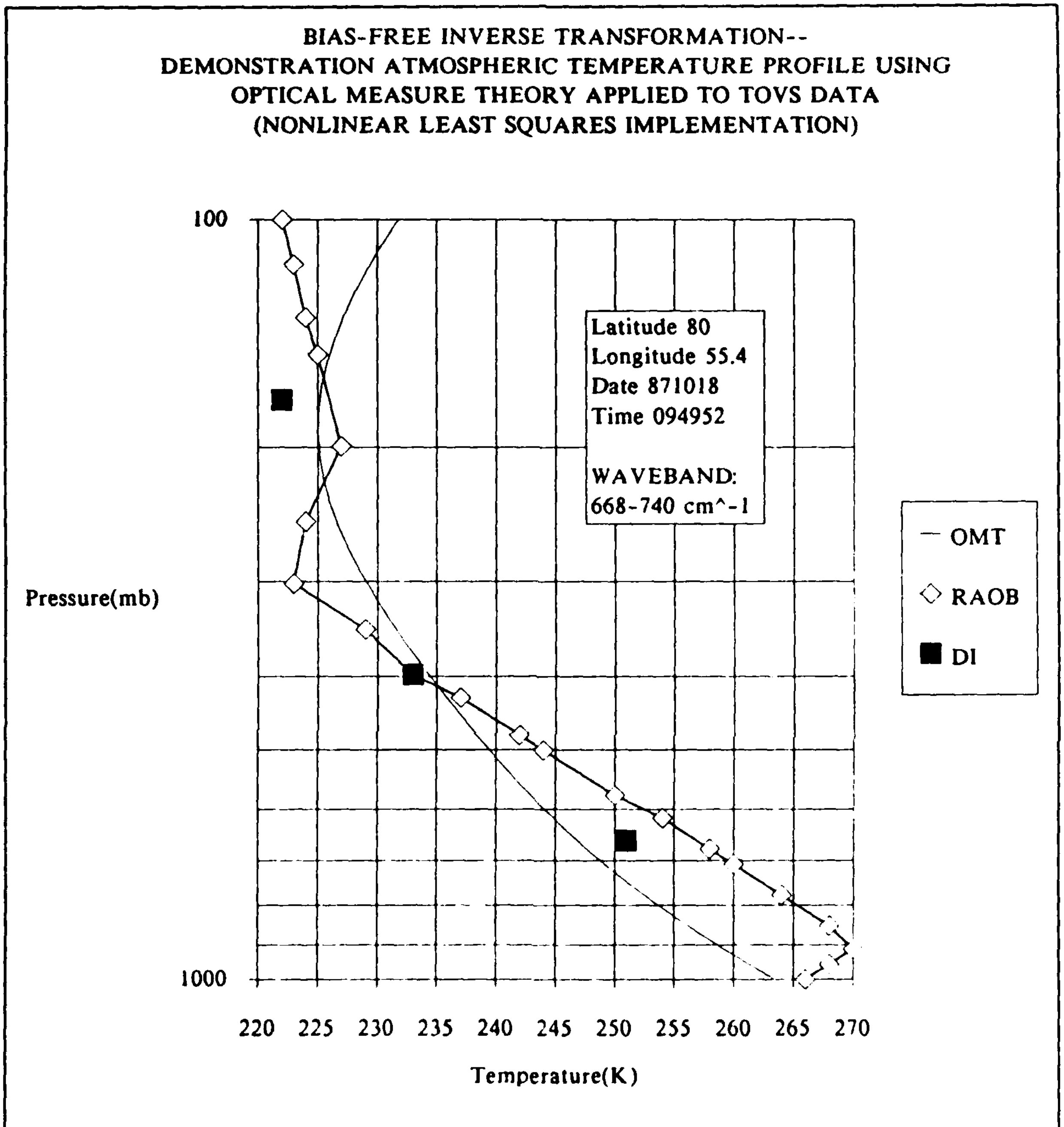

Figure 6. Comparison of Two Methods of Bias-Free Temperature Inversion. Shown is a comparison of temperature profiling methods implemented by Creative Optics, Inc.--Differential Inversion (DI) and Optical Measure Theory (OMT)--together with corresponding RAOB data. DI and OMT represent complementary bias-free methods for the determination of atmospheric temperatures. DI yields atmospheric temperatures with no assumption as to an underlying functional form, while OMT produces the smoothest temperature profile consistent with the radiance data. In conjunction, these two methods yield important new information on atmospheric temperatures from upwelling radiance data.

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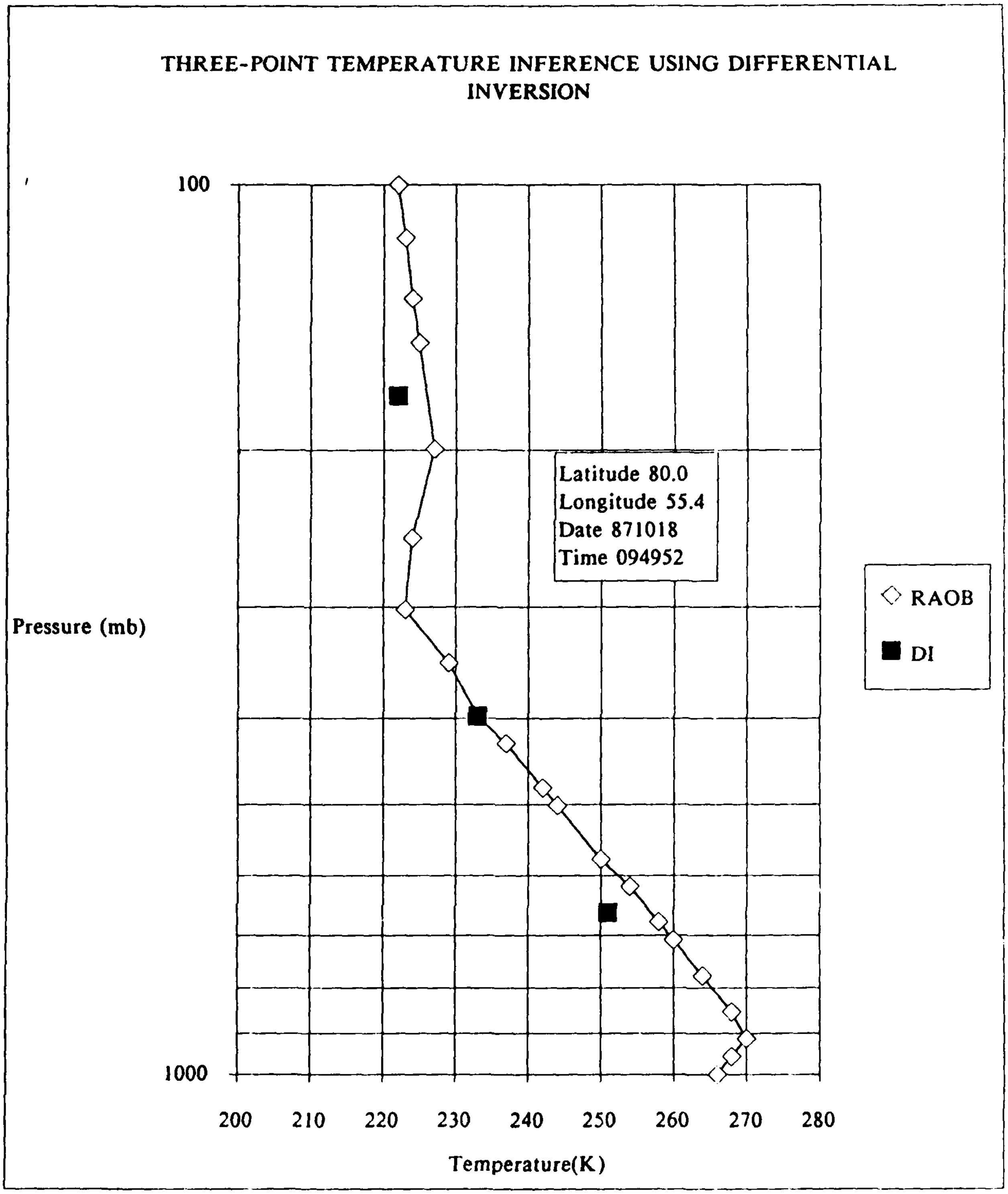
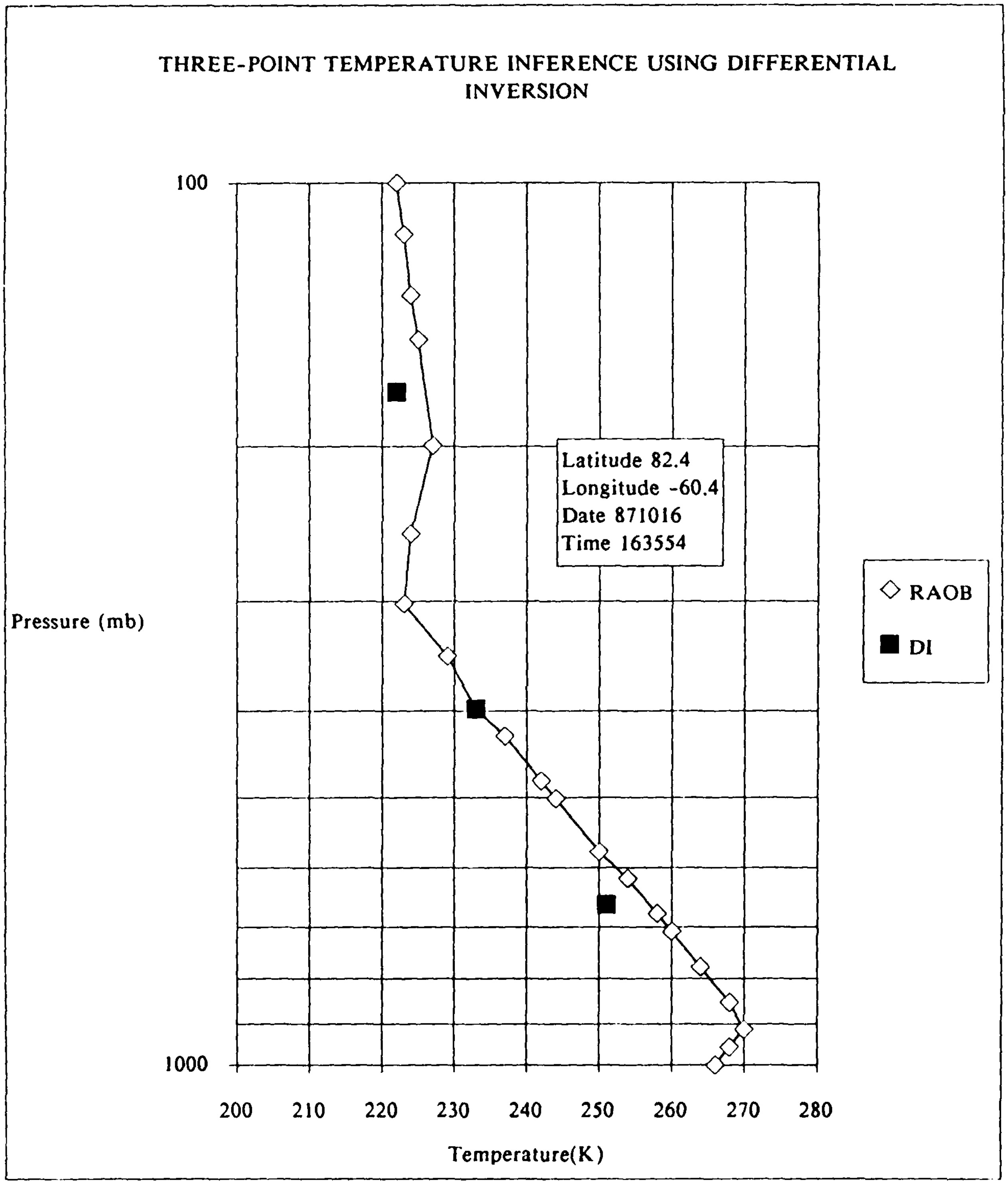
APPENDIX A

THREE-POINT TOVS TEMPERATURE INFERENCE USING DIFFERENTIAL INVERSION

We were able to determine temperatures from the TOVS data at three levels in the atmosphere in the 4.3μm wavelength band. The values of the pressure at these levels are 172.3, 400, 663 millibars. The figures are plots of the values for temperature from differential inversion together with RAOB measurements against pressure. The RAOB measurements are given by the solid line. Note that point on both sides of the tropopause were obtained



THREE-POINT TEMPERATURE INFERENCE USING DIFFERENTIAL INVERSION
100
1000
Pressure (mb)
Latitude 80.0
Longitude 55.4
Date 871018
Time 094952
RAOB
DI
200
210
220
230
240
250
260
270
280
Temperature(K)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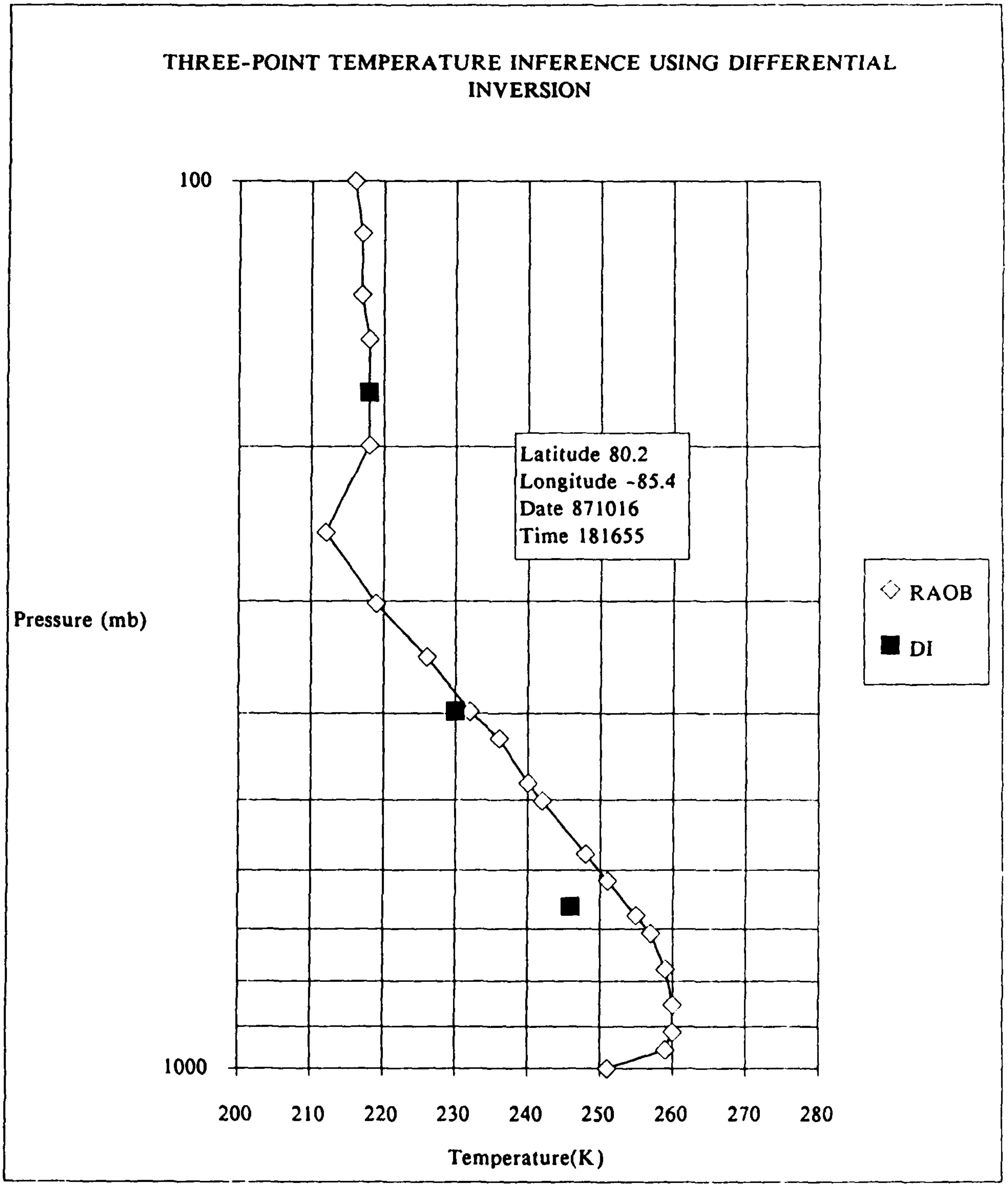
100
1000
Pressure (mb)
200
210
220
230
240
250
260
270
280
Temperature(K)
Latitude 82.4
Longitude -60.4
Date 871016
Time 163554
RAOB
DI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100
1000
Pressure (mb)
Latitude 80.2
Longitude -85.4
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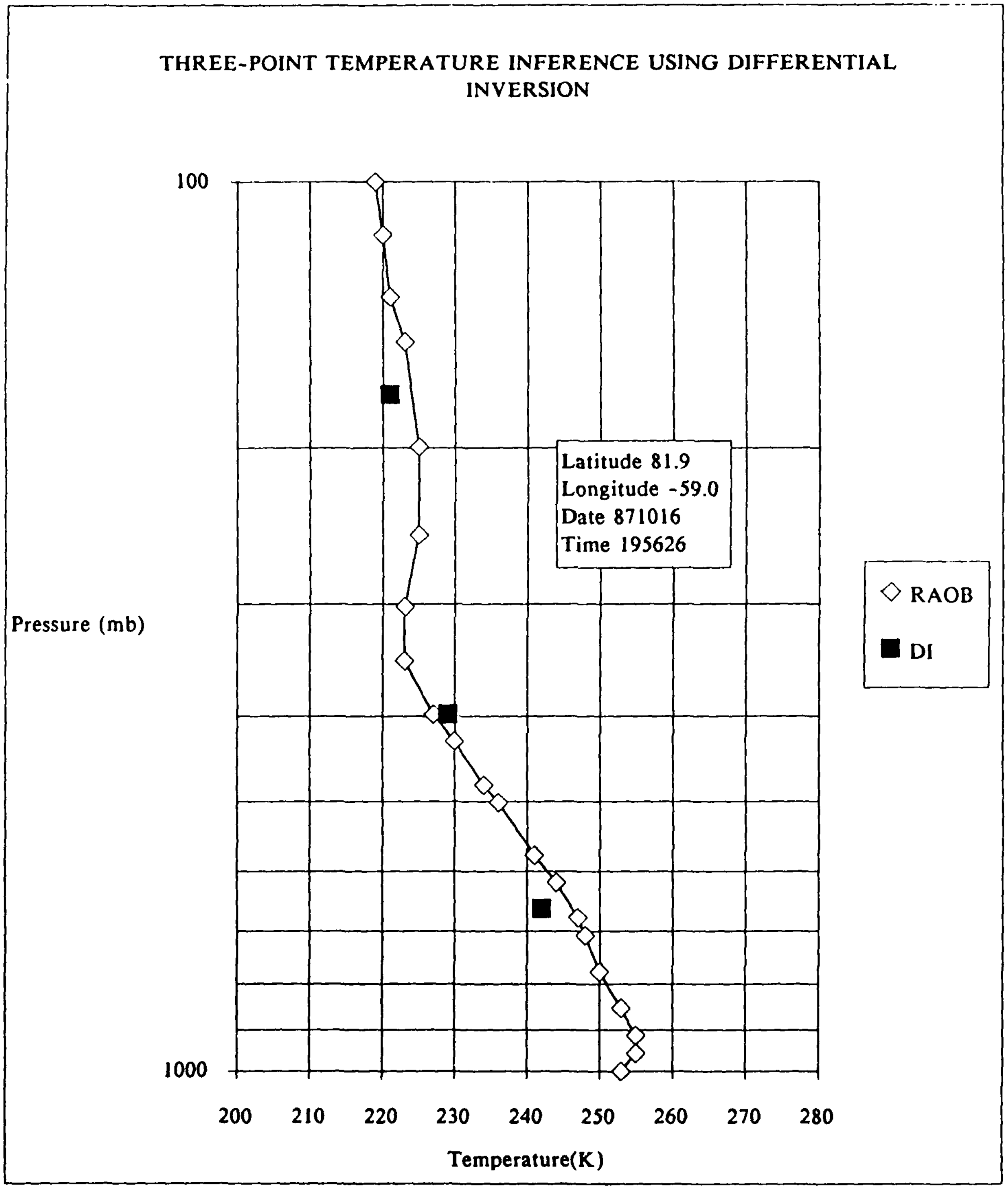
260
270
280
Temperature(K)



THREE-POINT TEMPERATURE INFERENCE USING DIFFERENTIAL INVERSION
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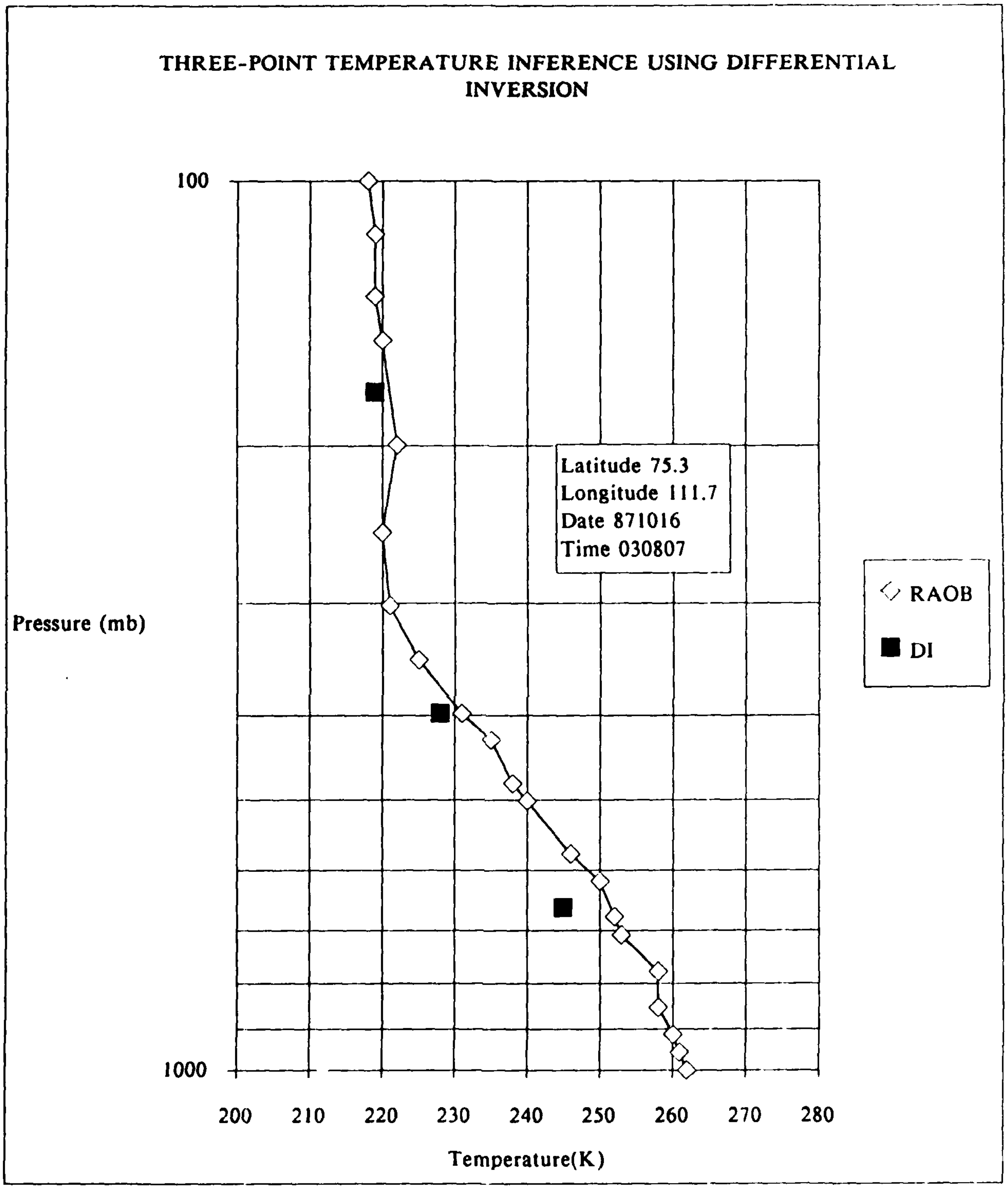
1000
Pressure (mb)
200
210
220
230
240
250
260
270
280
Temperature(K)
Latitude 81.9
Longitude -59.0
Date 871016
Time 195626
RAOB
DI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Pressure (mb)
200
210
220
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240
250
260
270
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Temperature(K)
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Longitude 111.7
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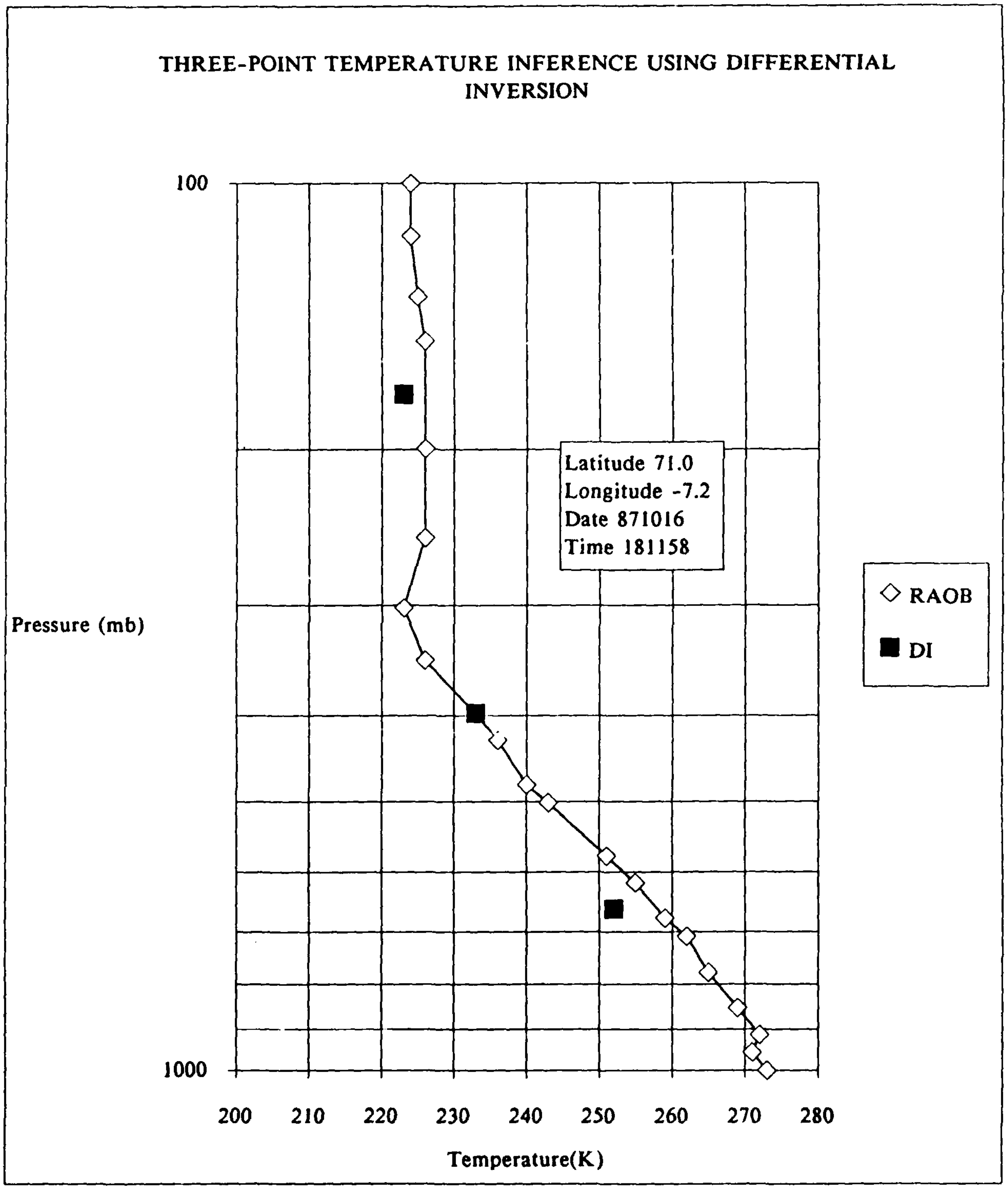
RAOB
DI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1000
Pressure (mb)
200
210
220
230
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260
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Temperature(K)
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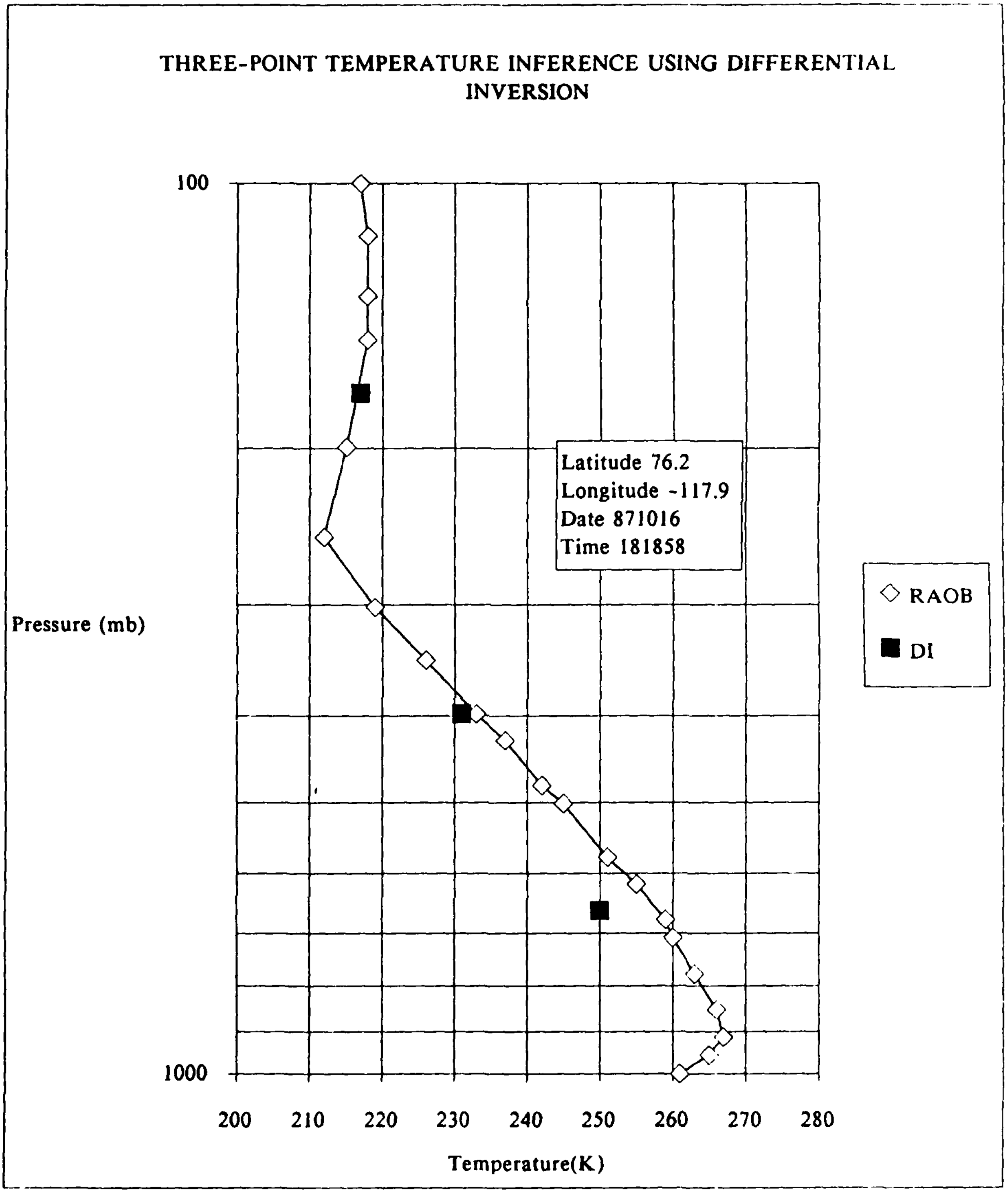
Date 871016
Time 181158
RAOB
DI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1000
Pressure (mb)
Latitude 76.2
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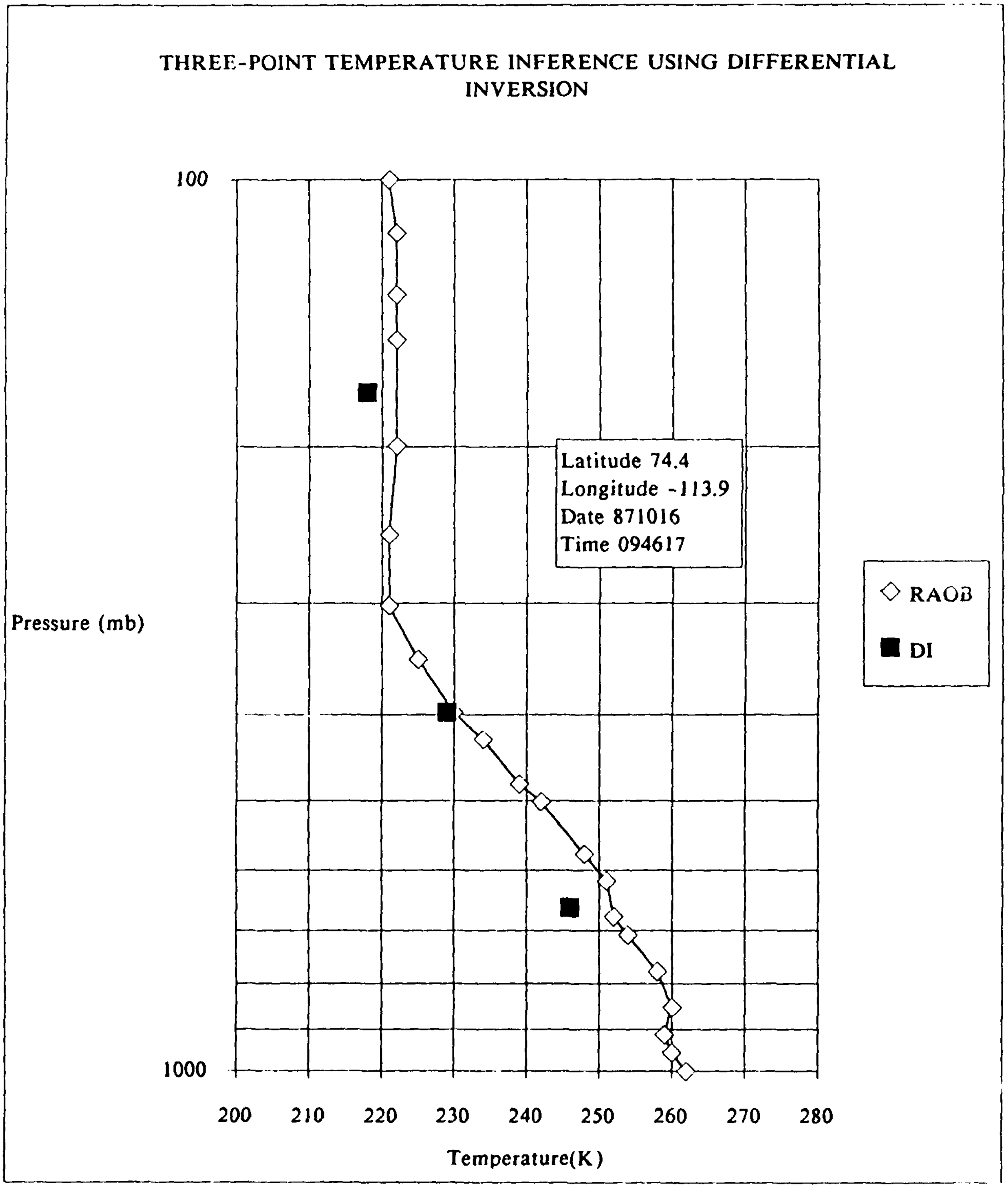
RAOB
DI
200
210
220
230
240
250
260
270
280
Temperature(K)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Pressure (mb)
200
210
220
230
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250
260
270
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Temperature(K)
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Longitude -113.9
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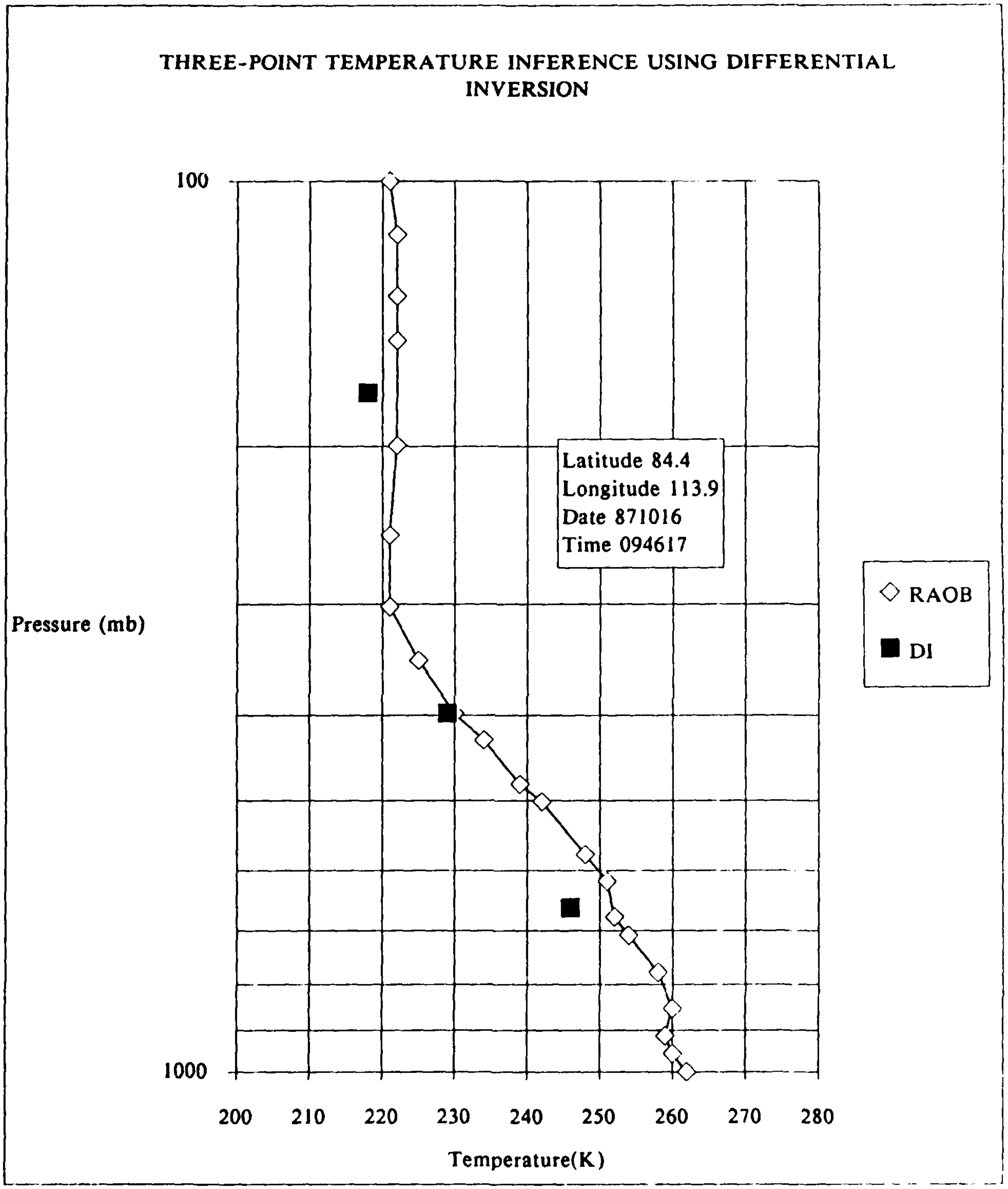
Time 094617
RAOB
DI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1000
Pressure (mb)
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210
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230
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260
270
280
Temperature(K)
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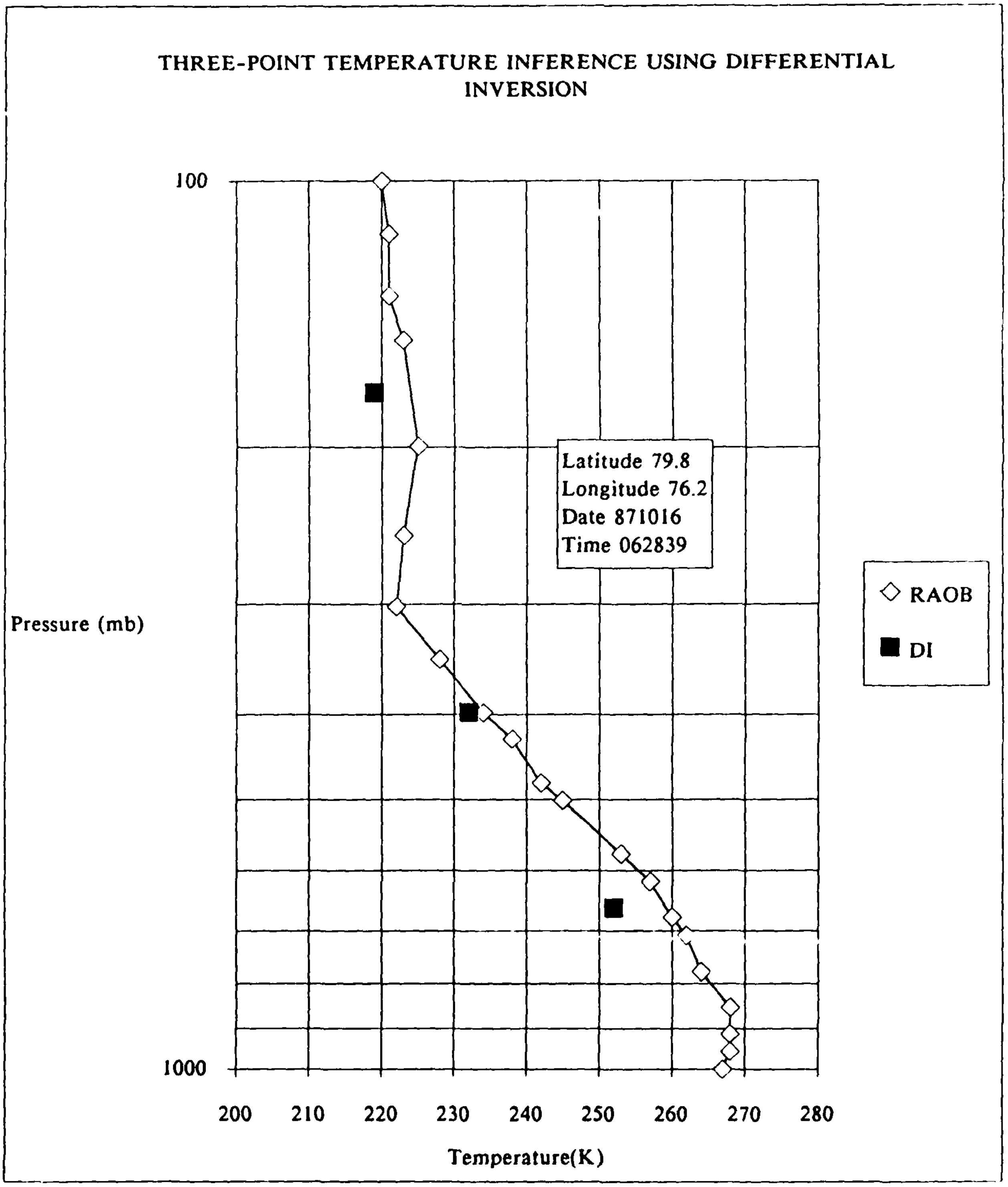
Time 094617
RAOB
DI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Pressure (mb)
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210
220
230
240
250
260
270
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Temperature(K)
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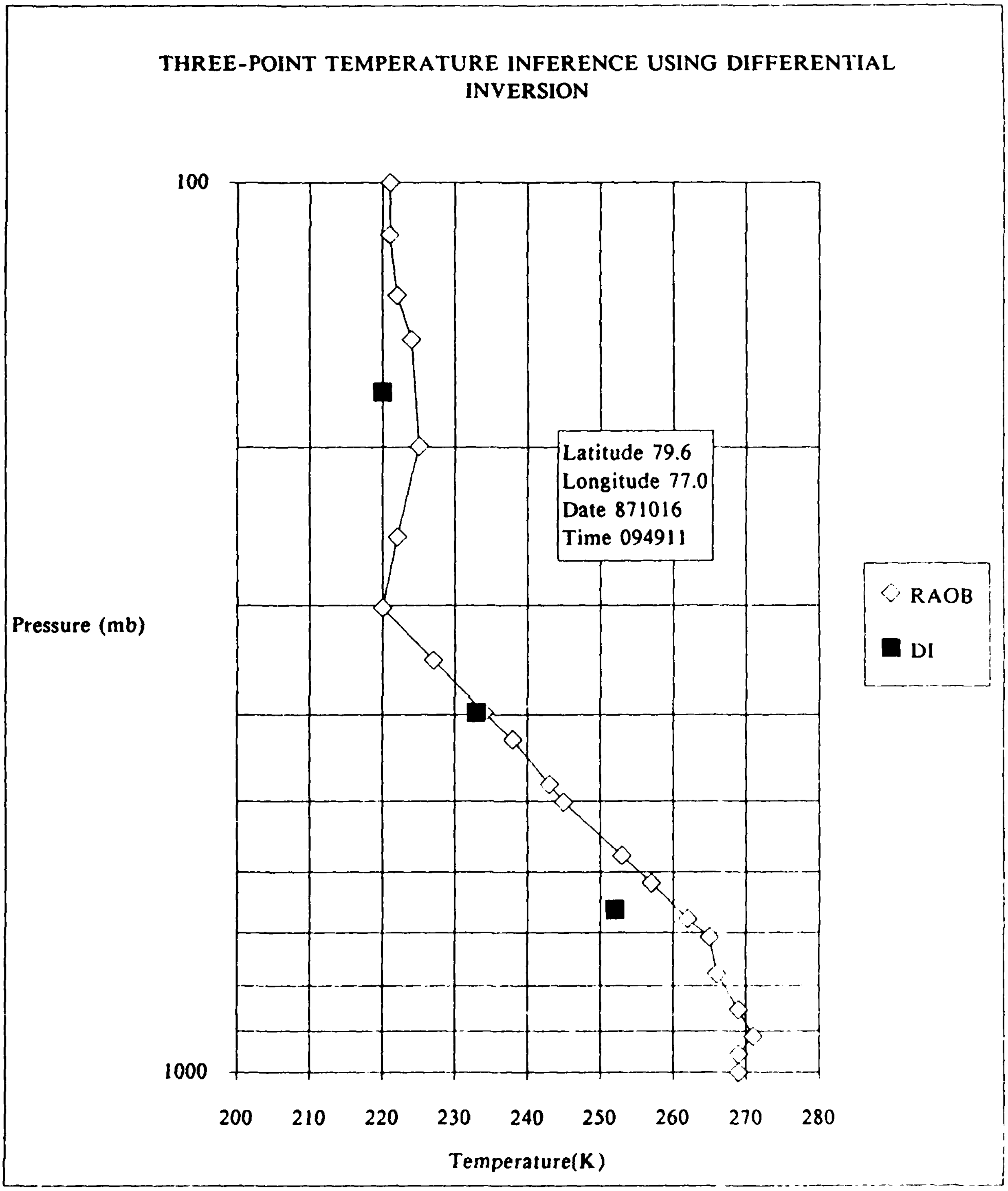
Date 871016
Time 062839
RAOB
DI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Pressure (mb)
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210
220
230
240
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260
270
280
Temperature(K)
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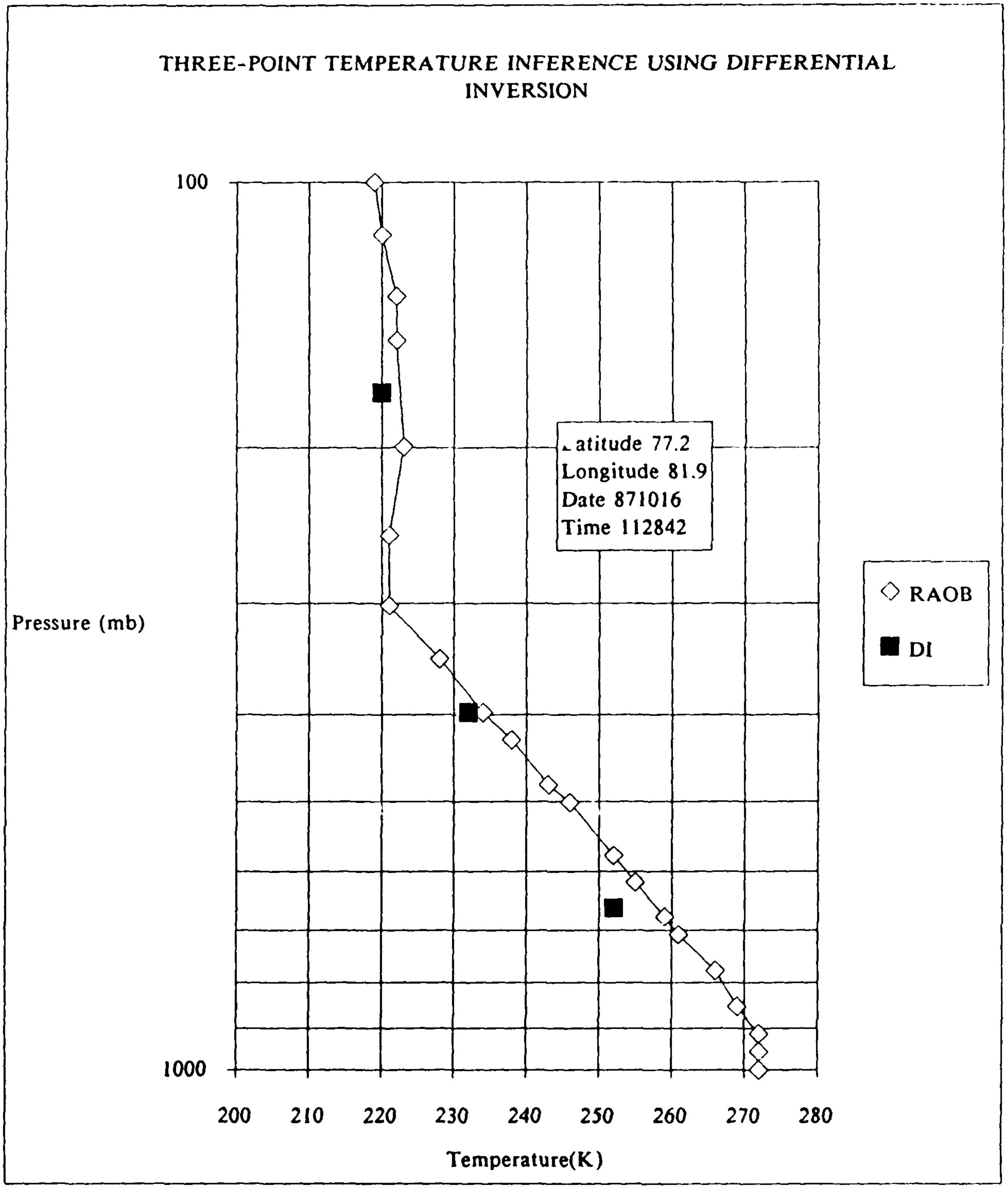
RAOB
DI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DI
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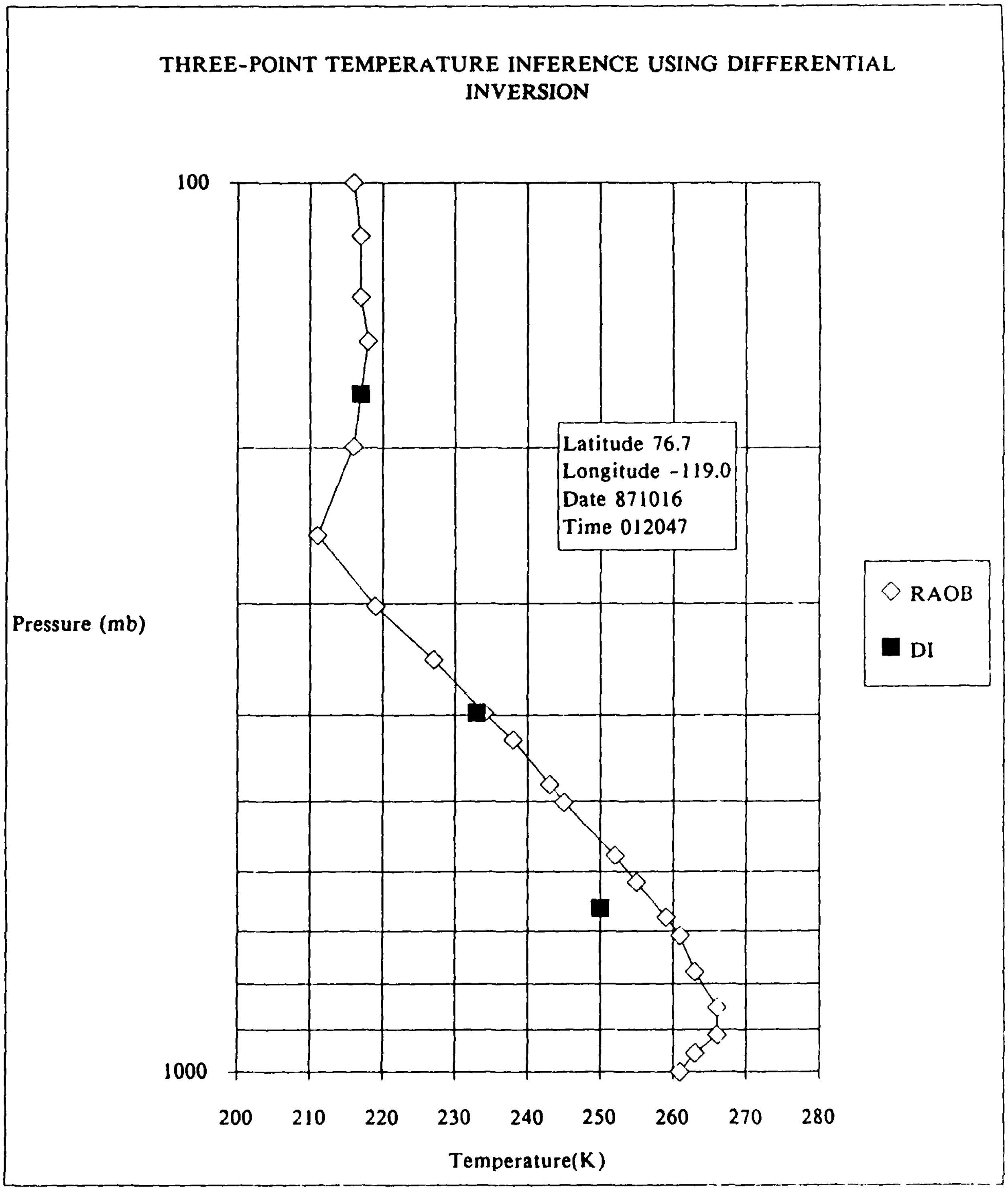
210
220
230
240
250
260
270
280
Temperature(K)



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1000
Pressure (mb)
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210
220
230
240
250
260
270
280
Temperature(K)
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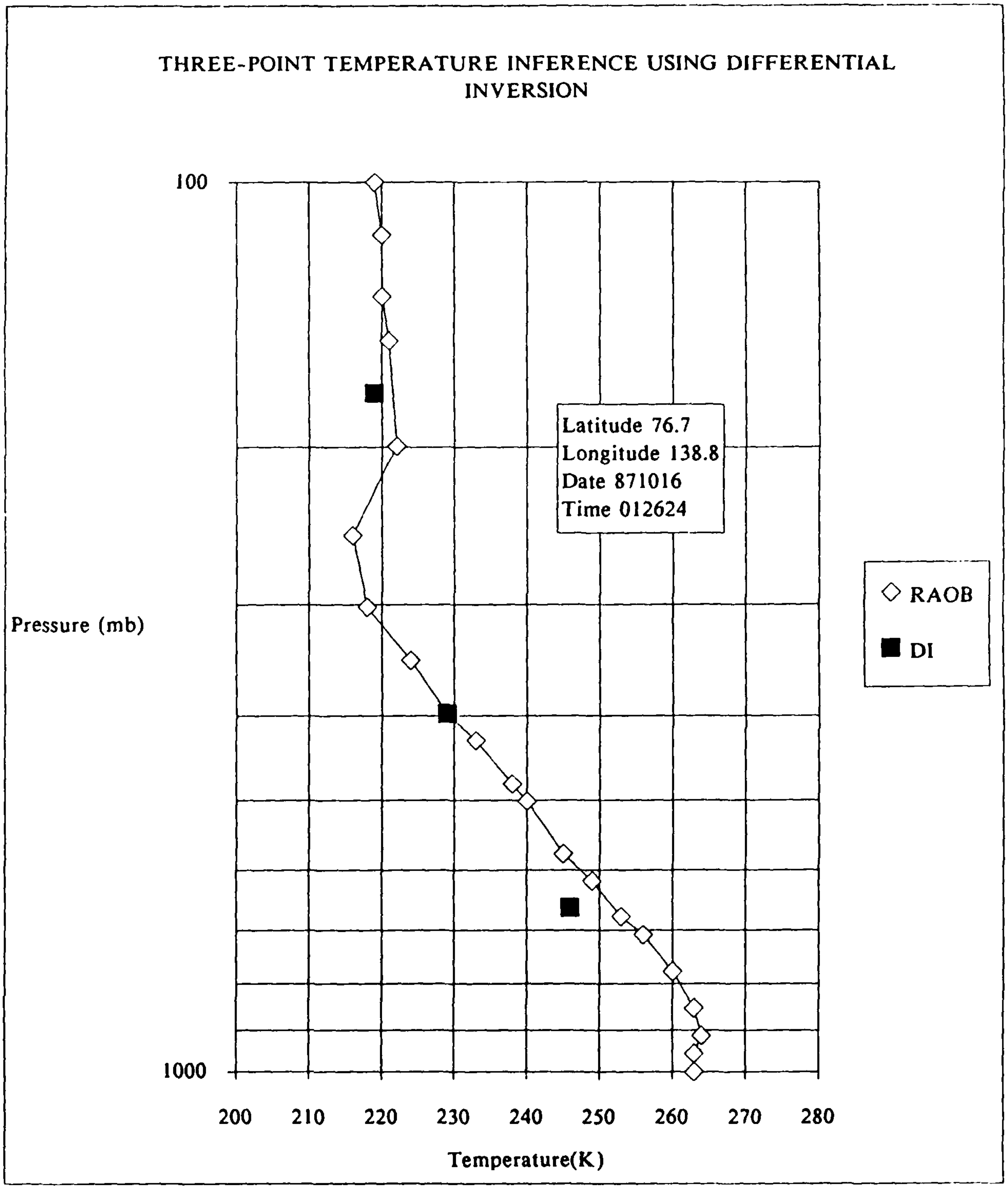
Time 012047
RAOB
DI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Pressure (mb)
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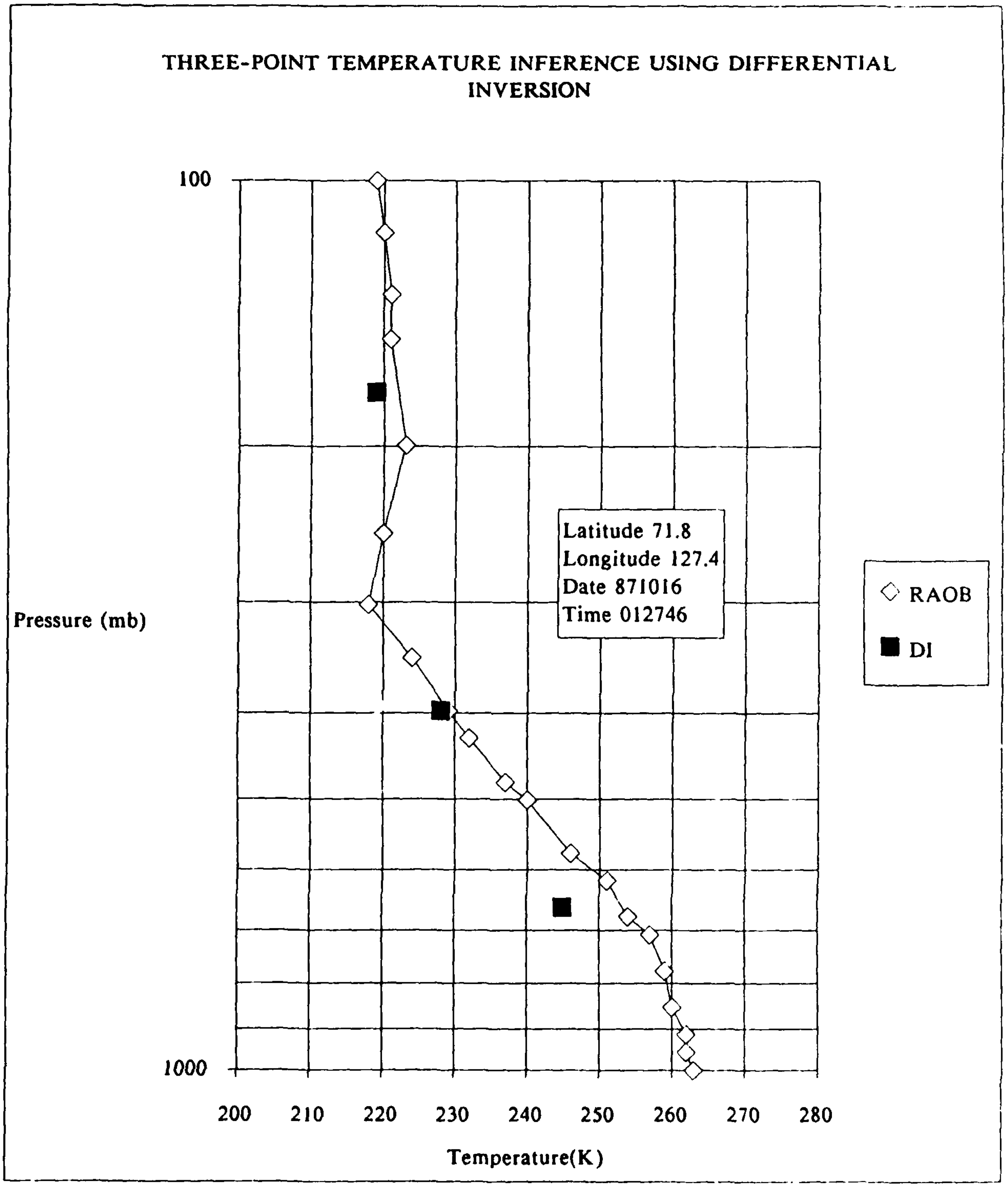
260
270
280
Temperature(K)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Pressure (mb)
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Longitude 127.4
Date 871016
Time 012746
RAOB
DI
200
210
220
230
240
250
260
270
280
Temperature(K)